```
     (FILE 'HOME' ENTERED AT 11:18:52 ON 27 JUN 2005)

     FILE 'CAPLUS' ENTERED AT 11:19:07 ON 27 JUN 2005
L1             STRUCTURE UPLOADED
               S L1

     FILE 'REGISTRY' ENTERED AT 11:19:31 ON 27 JUN 2005
L2          50 S L1

     FILE 'CAPLUS' ENTERED AT 11:19:32 ON 27 JUN 2005
L3           3 S L2
               S L1

     FILE 'REGISTRY' ENTERED AT 11:20:12 ON 27 JUN 2005
L4       21641 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 11:20:13 ON 27 JUN 2005
L5       13121 S L4 FULL
L6       10617 S L5 AND PY<1999
L7         927 S L6  AND (ESTER OR AMIDE)
L8         316 S L7 AND QUATERN?
L9          17 S L8 AND DICARBOXYLIC ACID

=>
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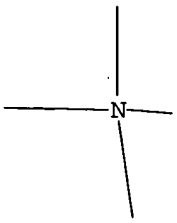
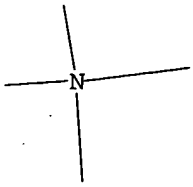
L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR





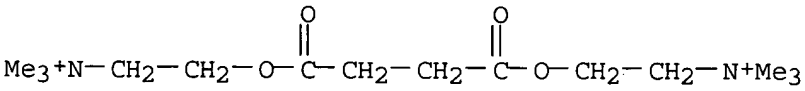
Structure attributes must be viewed using STN Express query preparation.

L9 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1989:205078 CAPLUS
DOCUMENT NUMBER: 110:205078
TITLE: Relations between structure, hydrolysis rate and activity of **dicarboxylic acid** esters
AUTHOR(S): Kharkevich, D. A.; Skoldinov, A. P.; Lemina, E. Yu.; Igumnova, N. D.
CORPORATE SOURCE: Dep. Pharmacol., First Med. Inst., Moscow, 119881, USSR
SOURCE: Farmakologiya i Toksikologiya (Moscow) (**1989**), 52(2), 34-7
CODEN: FATOAO; ISSN: 0014-8318
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB The kinetics of enzymic cholinesterase hydrolysis of **dicarboxylic acid** esters [MeN(R)-(CH2)n-O2C-(CH2)m-CO2-(CH2)n-(R)NMe + 2 MeI or 2 HCl, R = Me, 1-adamantyl; m = 1,2,4,6,8; n = 2,4] with neuromuscular-blocking activity was studied in vitro. The maximum hydrolysis rate was shown to increase on elongation of the distance between **ester** groups, both in the compds. containing a hydrophobic adamantyl radical attached to **quaternary** nitrogen, and in bis esters not containing adamantyl radicals. The comparison of neuromuscular-blocking activity in vivo, enzymic hydrolysis rates, and activity on isolated skeletal muscle demonstrated that in vivo activity is more strongly correlated with the maximum hydrolysis rate of the compds. than with activity in isolated skeletal muscle.

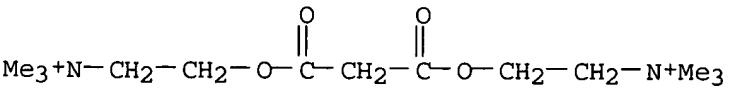
IT **541-19-5 1807-06-3 71677-28-6 71677-29-7 71677-30-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of, rate of, neuromuscular-blocking activity and structure in relation to)

RN 541-19-5 CAPLUS
CN Ethanaminium, 2,2'-[(1,4-dioxo-1,4-butanediyl)bis(oxy)]bis[N,N,N-trimethyl-, diiodide (9CI) (CA INDEX NAME)



●2 I⁻

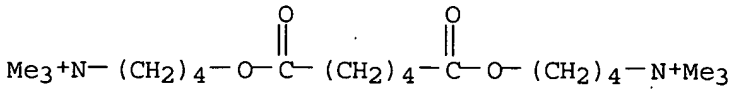
RN 1807-06-3 CAPLUS
CN Ethanaminium, 2,2'-[(1,3-dioxo-1,3-propanediyl)bis(oxy)]bis[N,N,N-trimethyl-, diiodide (9CI) (CA INDEX NAME)



●2 I⁻

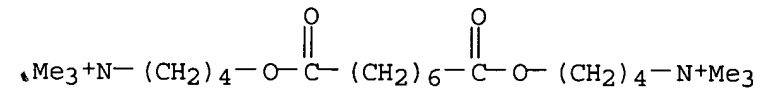
RN 71677-28-6 CAPLUS

CN 1-Butanaminium, 4,4'-[(1,6-dioxo-1,6-hexanediyl)bis(oxy)]bis[N,N,N-trimethyl-, diiodide (9CI) (CA INDEX NAME)



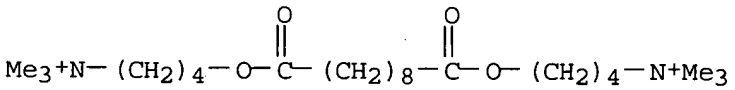
●2 I⁻

RN 71677-29-7 CAPLUS
CN 1-Butanaminium, 4,4'-[(1,8-dioxo-1,8-octanediyl)bis(oxy)]bis[N,N,N-trimethyl-, diiodide (9CI) (CA INDEX NAME)



●2 I⁻

RN 71677-30-0 CAPLUS
CN 1-Butanaminium, 4,4'-[(1,10-dioxo-1,10-decanediyl)bis(oxy)]bis[N,N,N-trimethyl-, diiodide (9CI) (CA INDEX NAME)



●2 I⁻

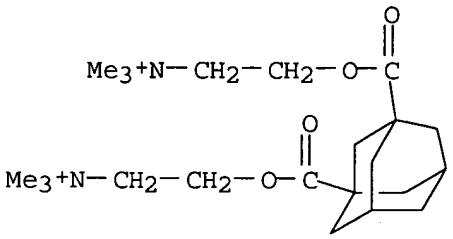
L9 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1974:520077 CAPLUS
DOCUMENT NUMBER: 81:120077
TITLE: Bis-**quaternary** ammonium salts containing an adamantyl radical
AUTHOR(S): Klimova, N. V.; Lavrova, L. N.; Skoldinov, A. P.; Kharkevich, D. A.; Shmar'yan, M. I.
CORPORATE SOURCE: Inst. Farmakol., Moscow, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (**1974**), 8(7), 3-5
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Reaction of I(CH2)nI (n 5, 6, 7) with RNMe2 (R = 1-adamantyl) gave 50-62.5% the corresponding Me2N+R(CH2)nN+-Me2R.2I- (I). I (n = 6) was a ganglion-blocking agent at 0.12-0.2 mg/kg in cats (hexonium = 40 mg/kg). Transesterification of di-Me 1,3-adamantanedicarboxylate with HO(CH2)2NMe2, followed by reaction of the resulting **ester** with MeI gave the bisammonium compound II. Reaction of 1,1'-diadamantyl-3,3'-**dicarboxylic acid** chloride with 1-methylpiperazine

followed by MeI gave the bispiperazinium salt III. III was an effective ganglion-blocking agent at 4-5 mg/kg in cats.

IT **51896-22-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and ganglion blocking activity of)

RN 51896-22-1 CAPLUS

CN Ethanaminium, 2,2'-[tricyclo[3.3.1.13,7]decane-1,3-diylbis(carbonyloxy)]bis[N,N,N-trimethyl-, diiodide (9CI) (CA INDEX NAME)



●2 I⁻

L9 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1973:92439 CAPLUS

DOCUMENT NUMBER: 78:92439

TITLE: Cyclobutane analogs of acetyl-γ-homocholine

AUTHOR(S): Cannon, Joseph G.; Lin, Youlin; Long, John Paul

CORPORATE SOURCE: Coll. Pharm., Univ. Iowa, Iowa City, IA, USA

SOURCE: Journal of Medicinal Chemistry (**1973**), 16(1), 27-9
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Cis-(2-acetoxycyclobutylmethyl)trimethylammonium iodide (cis-I) [38868-89-2] and trans-(2-acetoxycyclobutylmethyl)trimethylammonium iodide (trans-I) [38868-90-5] had 40,000-fold and 5000-fold lower muscarinic activity, resp., than acetylcholine [51-84-3] in the superfused guinea pig ileum in vitro. The effects of both were blocked by atropine [51-55-8] but not by hexamethonium [**60-26-4**]. To synthesize cis-I, cis-cyclobutane-1,2-**dicarboxylic acid** mono-Me **ester** [31420-52-7] was converted with SOCl2 to the mono-Me **ester** monoacyl chloride, with Me2CD to the mono-Me **ester** Me ketone, and with m-chloroperbenzoic acid to Me cis-2-acetoxycyclobutanecarboxylate [38868-92-7]. Aminolysis with NHMe2 gave a mixture of products which was reduced with LiAlH4 to cis-2-dimethylaminomethylcyclobutanol [38868-93-8]. This was **quaternized** with MeI and acetylated to yield cis-I. Trans-I was synthesized similarly.

IT **60-26-4**
RL: BIOL (Biological study)
(parasympathomimetic effects of acetyl homocholine derivs. in response to)

RN 60-26-4 CAPLUS

CN 1,6-Hexanediaminium, N,N,N,N',N',N'-hexamethyl- (9CI) (CA INDEX NAME)

$Me_3{}^+N-(CH_2)_6-N^+Me_3$

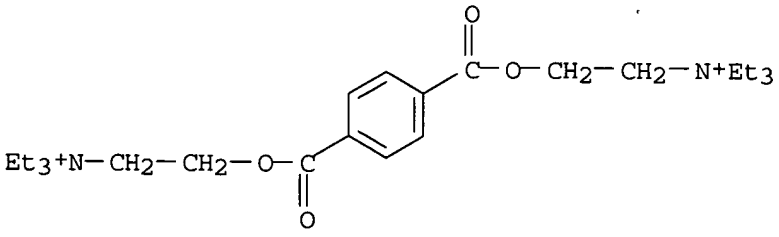
L9 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1972:140248 CAPLUS
DOCUMENT NUMBER: 76:140248
TITLE: Glycol esters
INVENTOR(S): Kamatani, Hiroyoshi
PATENT ASSIGNEE(S): Toyo Spinning Co., Ltd.
SOURCE: Jpn. Tokkyo Koho
CODEN: JAXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 47002623	B4	19720125	JP	19680924 <--

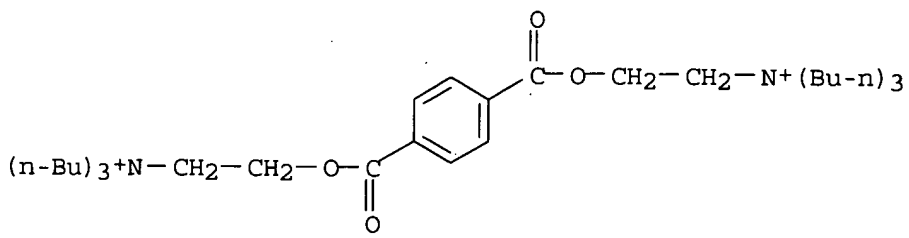
AB An aromatic **dicarboxylic acid** was made to react with an alkylene oxide, with use of a **quaternary** ammonium aromatic carboxylate having at least 1 N-(2-hydroxyalkyl) group as a catalyst. E.g., terephthalic acid was heated 100 min at 120° with ethylene oxide in xylene using 0.3 molar % bis(2-hydroxyethyltriethylammonium) terephthalate as a catalyst to give 75% **ester**. Examples of other catalysts used are bis(2-hydroxyethyltributylammonium) terephthalate and mono-(2-hydroxyethyldiethylcyclohexylammonium) terephthalate.

IT **35719-59-6 35719-60-9**
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for esterification of terephthalic acid by ethylene oxide)

RN 35719-59-6 CAPLUS
CN Ethanaminium, 2,2'-[1,4-phenylenebis(carbonyloxy)]bis[N,N,N-triethyl- (9CI) (CA INDEX NAME)



RN 35719-60-9 CAPLUS
CN 1-Butanaminium, N,N'-[1,4-phenylenebis(carbonyloxy-2,1-ethanediyl)]bis[N,N-dibutyl- (9CI) (CA INDEX NAME)



L9 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1968:486735 CAPLUS
DOCUMENT NUMBER: 69:86735
TITLE: Acetylcholine. XII. 3,4-Diphenylthiophene-2.5-

dicarboxylic acid bis [(β-diethylamino)ethyl **ester** methiodide], a curarelike muscle-relaxant **ester**

AUTHOR(S): Dann, O.; Bamberg, K. J.; Sucker, H.
CORPORATE SOURCE: Univ. Erlangen-Nuernberg, Erlangen-Nuernberg, Fed. Rep. Ger.

SOURCE: Pharmazie (**1968**), 23(3), 135-45
CODEN: PHARAT; ISSN: 0031-7144
DOCUMENT TYPE: Journal
LANGUAGE: German

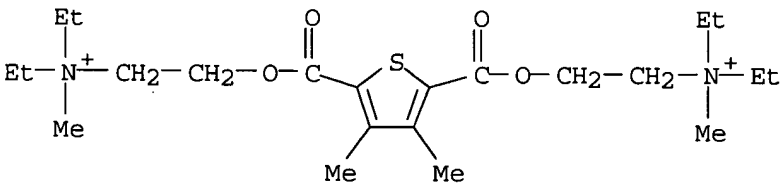
GI For diagram(s), see printed CA Issue.

AB The muscle-relaxing properties of **quaternized** amino alc. esters of 3,4-diphenyl- (I), 3,4-dimethyl- (II), 3,4-di(2-furyl)- (III), and 3,4-bis(5-nitro-2-furyl)thiophene-2,5-**dicarboxylic acid** (IV); phenanthreno[9,10-c]thiophene-1,3-**dicarboxylic acid** (V); and 2,3-diphenylbenzene-1,4- (VI), 3,6-diphenylbenzene-1,2- (VII), and 2,5-diphenylfuran-3,4-**dicarboxylic acid** (VIII) were determined I (10 g.) was boiled with 300 ml. $SOCl_2$ and worked up to give 8.1 g. I dichloride (IX), m. 123-4°. Similarly prepared were 37% II dichloride (X), m. 67-73°; III dichloride (XI), 91%, m. 90.5-1.5° (ligroine); IV dichloride, m. 92.5-95° (C_6H_6); V dichloride (XII), 37%, m. 193-4° (C_6H_6); and VI dichloride (XIII), 80%, m. 153.5-56° (decomposition) (ligroine). VIII (5.5 g.) was added in small portions with stirring to an ice-cold suspension of 16 g. PCl_5 in 55 ml. Et_2O, stirred 30 min., and worked up to give 4.8 g. VIII dichloride (XIV), m. 120-1° (twice from ligroine). Crude II in dioxane was treated with CH_2N_2 in Et_2O, kept 3 hrs., and worked up to give 36% di-Me **ester**, m. 171.5-2.5° (also prepared by heating X and MeOH), which was refluxed in methanolic KOH and worked up to give pure II, decompose 324-7°. Similarly, III (at -5°), gave 90% di-Me **ester**, m. 129° (twice from AcOH), which, at -5° in Ac_2O, was nitrated with HNO_3 (d. 1.52), stirred 1 hr., and worked up to give IV di-Me **ester**, m. 182-4°, which refluxed 2 min. in methanolic KOH and worked up gave IV, m. 258° (decomposition). A suspension of 2 g. 1,4-dimethyl-2,3-diphenylbenzene in 60 ml. C_5H_5N and 20 ml. H_2O containing 25.3 g. $KMnO_4$ was refluxed 2 hrs. and worked up to give 2.2 g. VI, m. 308-11°. IX (15.6 g.) and 25.2 g. β-diethylaminoethanol (DEAE) was refluxed 6 hrs. in 500 ml. dry C_6H_6 and worked up to give 14.8 g. I bis(β-diethylaminoethyl **ester**), m. 76.5-77° (ligroine); dipicrate m. 175.5-77° (1:1 Me_2CO-H_2O); di-HBr salt m. 185.5-6.5° (Me_2CO-iso-PrOH); dimethiodide m. 212-13° (decomposition); bis(benzyl bromide) decomposed 191°, m. 240-7° (EtOH-EtOAc). The following were prepared II bis(β-diethylaminoethyl **ester**), 70% [di-HBr salt m. 212.5-14° (decomposition); dimethiodide m. 202.5-2.5° (decomposition)]; III bis(β-diethylaminoethyl **ester**), 61%, n22D 1.459, by shaking XI and DEAE in C_6H_6 66 hrs. at room temperature and working up [di-HBr salt, m. 179.5-81° (decomposition); dimethiodide m. 177.5-79° (decomposition)]; IV bis(β-diethylaminoethyl **ester**), 47%, m. 42-7° (dimethiodide m. 192-5°); VI bis(β-diethylaminoethyl **ester**), 62%, n22D 1.540 [di-HBr salt m. 185.5-7.5° (EtOAc:EtOH); dimethiodide, m. 234-5° (decomposition)]; VIII bis(β-diethylaminoethyl **ester**), 74% [di-HBr salt m. 180-1° (3:1 Me_2CO-EtOH); dimethiodide m. 185.5-87° (decomposition)] I bis(β-dimethylaminoethyl **ester**) 65%, m. 69-79° (ligroine) [dimethiodide decomposed 225-50° (EtOH)]; and V bis(β-diethylaminoethyl **ester**), 90%, [di-HCl salt, decompose 211-12.5°; dimethiodide m. 215-16° (decomposition)]. XII (1.25 g.) and 1.1 g. MeOH refluxed in 5 ml. C_6H_6 and cooled precipitated 0.85 g. V di-Me **ester**, m. 118-19°. DEAE (4.7 g.) in 50 ml. Me_2CO was added to 12 g. VII anhydride suspended in 250

ml. dry refluxing Me2CO, and the mixture refluxed 20 min. to precipitate 14.6 g. of the half **ester**, m. 205-22°, difficulty soluble in 2N NaOH and 2N HCl. This intermediate (8.35 g.) and 5.4 g. β-diethylaminoethyl chloride was refluxed 6.5 hrs. in 160 ml. dry iso-PrOH and worked up to give 7.3 g. VII bis(β-diethylaminoethyl **ester**), m. 99-100° (ligroine and petroleum ether); di-HBr salt m. 193-5°; dimethiodide m. 206.5-7.5° (decomposition). The anhydride (5 g.) of cis, cis, cis,cis-3,6-diphenyl-1,2,3,6-tetrahydrobenzene-1,2-**dicarboxylic acid** in 80 ml. HCONMe2 was hydrogenated at atmospheric pressure and room temperature over Pd(OH)2 on BaSO4 and worked up to give 3.3 g. anhydride of cis, cis, cis, cis-3,6-diphenylcyclohexane-1,2-**dicarboxylic acid**, m. 220-2° (EtOAc). A solution of 4.8 g. 2,7-diaminodiphenylene sulfone and 14 g. di-Et diacetylsuccinate in 20 ml. AcOH was refluxed 45 min. and cooled to precipitate 12.5 g. XV, m. 251-3° (BuOH:AcOH), saponified to the free acid by methanolic KOH. A mixture of 1.28 g. 2,2'-dihydroxy-5,5'-dimethyldeoxybenzoin in 2N NaOH and 1 g. ClCH2CO2H solution neutralized with K2CO3 was refluxed 3 hrs. and worked up to give 2-hydroxy-2'-carboxymethoxy-5,5'-dimethyldeoxybenzoin, m. 159-61° (60% EtOH), and 2,2'-dicarboxymethoxy-5,5'-dimethyldeoxybenzoin, m. 172-4° (60% AcOH and 60% EtOH). Extensive biol. data are given.

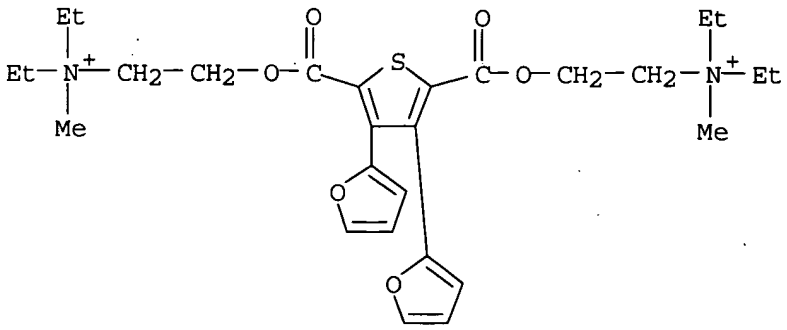
IT **19799-17-8P 19799-21-4P 19799-34-9P 19799-36-1P 19802-94-9P 19802-96-1P 19971-00-7P 19976-53-5P 19976-55-7P 20653-69-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 19799-17-8 CAPLUS
CN Ammonium, diethyl(2-hydroxyethyl)methyl-, iodide, 3,4-dimethyl-2,5-thiophenecarboxylate (2:1) (8CI) (CA INDEX NAME)



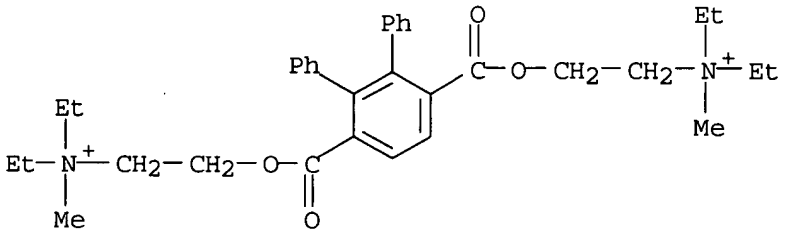
●2 I⁻

RN 19799-21-4 CAPLUS
CN Ammonium, diethyl(2-hydroxyethyl)methyl-, iodide, 3,4-di-2-furyl-2,5-thiophenedicarboxylate (2:1) (8CI) (CA INDEX NAME)



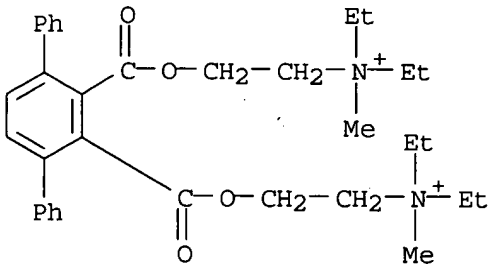
●2 I^-

RN 19799-34-9 CAPLUS
CN Ammonium, diethyl(2-hydroxyethyl)methyl-, iodide, [o-terphenyl]-3',6'-dicarboxylate (2:1) (8CI) (CA INDEX NAME)



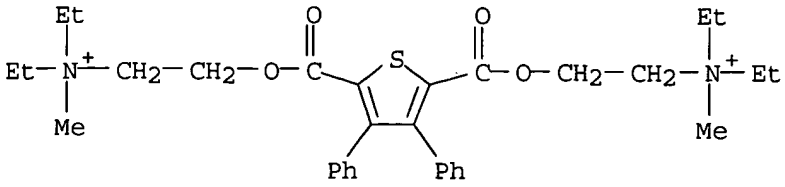
●2 I^-

RN 19799-36-1 CAPLUS
CN Ammonium, diethyl(2-hydroxyethyl)methyl-, iodide, [p-terphenyl]-2',3'-dicarboxylate (2:1) (8CI) (CA INDEX NAME)



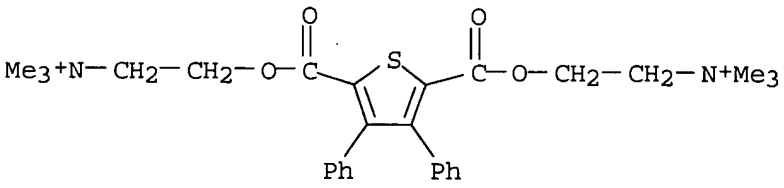
●2 I^-

RN 19802-94-9 CAPLUS
CN Ammonium, diethyl(2-hydroxyethyl)methyl-, iodide, 3,4-diphenyl-2,5-thiophenedicarboxylate (2:1) (8CI) (CA INDEX NAME)



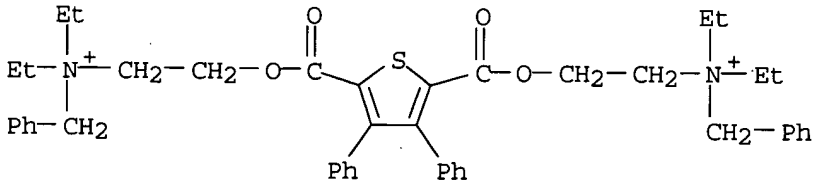
●2 I^-

RN 19802-96-1 CAPLUS
CN Choline, iodide, 3,4-diphenyl-2,5-thiophenedicarboxylate (2:1) (8CI) (CA INDEX NAME)



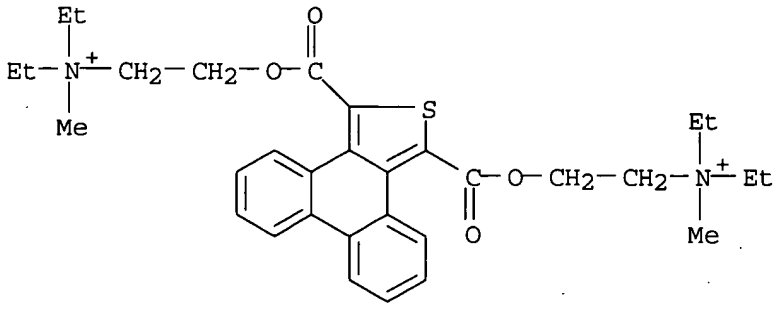
●2 I^-

RN 19971-00-7 CAPLUS
CN Ammonium, benzyldiethyl(2-hydroxyethyl)-, bromide, 3,4-diphenyl-2,5-thiophenedicarboxylate (2:1) (8CI) (CA INDEX NAME)



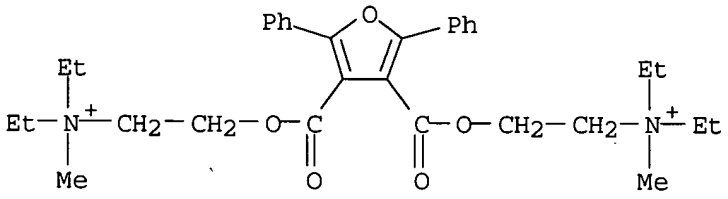
●2 Br^-

RN 19976-53-5 CAPLUS
CN Ammonium, diethyl(2-hydroxyethyl)methyl-, iodide, phenanthro[9,10-c]thiophene-1,3-dicarboxylate (2:1) (8CI) (CA INDEX NAME)



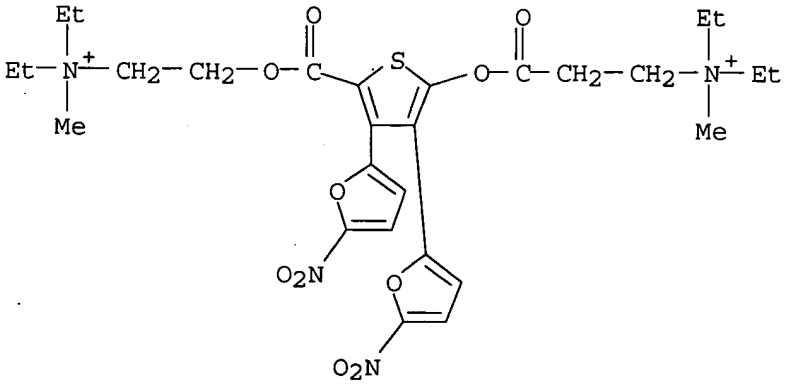
●2 I⁻

RN 19976-55-7 CAPLUS
CN Ammonium, diethyl(2-hydroxyethyl)methyl-, iodide, 2,5-diphenyl-3,4-furandicarboxylate (2:1) (8CI) (CA INDEX NAME)



●2 I⁻

RN 20653-69-4 CAPLUS
CN Ammonium, diethyl(2-hydroxyethyl)methyl-, iodide, 3,4-bis(5-nitro-2-furyl)-2,5-thiophenedicarboxylate (2:1) (8CI) (CA INDEX NAME)



●2 I⁻

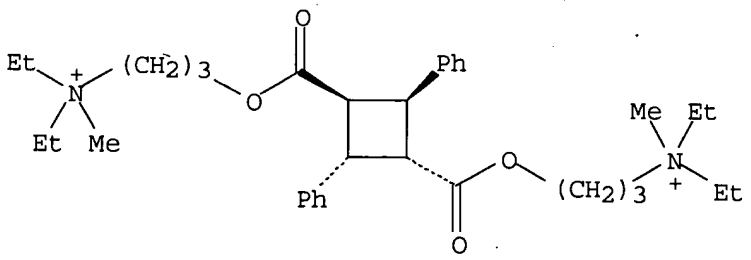
L9 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1968:401562 CAPLUS

DOCUMENT NUMBER: 69:1562
TITLE: Cyclobutanedicarboxylic acids. VI. Relation between curariform activity and structure in a series of alkamine cyclobutanedicarboxylic acid derivatives
AUTHOR(S): Kharkevih, D. A.; Arendaruk, A. P.; Skoldinov, A. P.
CORPORATE SOURCE: Mosk. Med. Inst. im. Sechenova, Moscow, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (**1968**), 2(3), 7-11
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB The curariform activity of a series of alkamine cyclobutane **dicarboxylic acid** derivs. was determined by drooping head symptom in rabbits and by a study of the effect of the compds. on the transfer of stimulation from the sciatic nerve to the gastrocnemius muscle of cats. Activity was studied in relation to 4 structural features: distance between the **quaternary** N atoms, radicals shielding these N atoms, stereoconfiguration of the truxillic acids, and the structure of the aliphatic part of the mol. separating the 2 **quaternary** N atoms. The bis(N-methylpiperidino)cyclobutanedicarboxylates and bis(diethylmethylammonium)cyclobutanedicarboxylates with 11 C and 2 O atoms between the 2 **quaternary** groups were the most effective curariform agents. The α-truxillic acid derivs. were the most effective and the γ-truxillic acid derivs. the least effective in suppressing transfer of nerve impulses. Replacement of **ester** groups with amides increased the curariform activity of the diphenylcyclobutanedicarboxylic acid bisquaternary ammonium salts. These compds. apparently are antidepolarizing curariform substances which interact with only 1 choline receptor. 21 references.

IT **4304-01-2**
RL: BIOL (Biological study)
(neuromuscular transmission inhibition by)
RN 4304-01-2 CAPLUS
CN 1-Propanaminium, 3,3'-[[(1α,2α,3β,4β)-2,4-diphenyl-1,3-cyclobutanediyl]bis(carbonyloxy)]bis[N,N-diethyl-N-methyl-, diiodide (9CI) (CA INDEX NAME)

Relative stereochemistry.



●2 I⁻

L9 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1966:465269 CAPLUS
DOCUMENT NUMBER: 65:65269
ORIGINAL REFERENCE NO.: 65:12122d-f
TITLE: Bischoline esters of bicyclic dicarboxylic acids and related compounds
AUTHOR(S): Koch, H.; Kotlan, J.
CORPORATE SOURCE: Univ., Vienna

SOURCE: Monatshefte fuer Chemie (**1965**), 96(6), 2000-4
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: German

GI For diagram(s), see printed CA Issue.

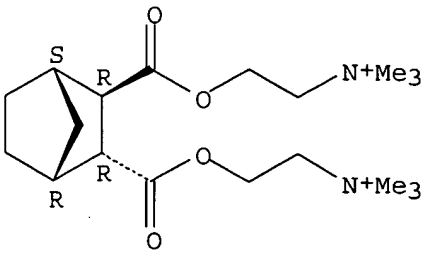
AB The Me **ester** of bicyclo[2.2.1]heptane- and bicyclo[2.2.2]octane-trans-dicarboxylic acids and their unsatd. analogs (I-IV) were prepared by Diels-Alder reaction. The esters and dialkylamino alcs. gave basic esters A (R= CHR2CH2R1), which were converted to dihydrochlorides B (R = CHR2CH2R1.HCl) and bis(**quaternary** ammonium salts) C (R = CHR2CH2R1.R3X) in the usual manner. The compds. prepared are given in the table. Some of the compds. are muscle-relaxants. C (m.p.); R1, R2, A (b.p./mm.), B (m.p.), a, b; I, NMe2, H, 180-90°/2, 203-5°, 234-6°, 197-9°;I, NMe2, Me, 185-95°/5, 215-17°, 219-21°, oil, I; NEt2, H, 205-15°/5, 133-5°, oil, 173-5°; I piperidino, H, 205-20°/5, 227-9°, 184-7°, 96-9°; II NMe2, H, 185-95°/2, 179-82°, 235-8°,194-6°; II NEt2 H, 210-15°/2, 165-8°, -, 204-9°; III NMe2, H, 180-90°/2, 198-201°, 210-13°, 174-7°; III NMe2, Me, 190-200°/5, 231-3°, 179-82°, oil; III NEt2, H, 210-20°/5, 158-60°, oil, -;IV, NMe2, H, 185-90°/2, 175-80°, 208-11°, 217-21°; a:, R3X, =, MeI, b:, R3X, =, EtBr.;

IT **5783-18-6**, Choline, iodide, 2,3-norbornanedicarboxylate, trans- **7172-48-7**, Ammonium, ethyl(2-hydroxypropyl)dimethyl, bromide, 5-norbornene-2,3-dicarboxylate, trans- **10491-44-8**, Choline, iodide, bicyclo[2.2.2]octane-2,3-dicarboxylate, trans- (preparation of)

RN 5783-18-6 CAPLUS

CN Ethanaminium, 2,2'-[bicyclo[2.2.1]heptane-2,3-diylbis(carbonyloxy)]bis[N,N,N-trimethyl-, diiodide, (2-endo,3-exo)- (9CI) (CA INDEX NAME)

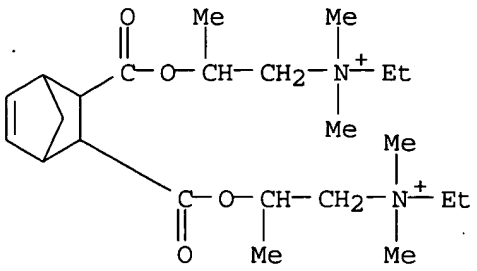
Relative stereochemistry.



●2 I⁻

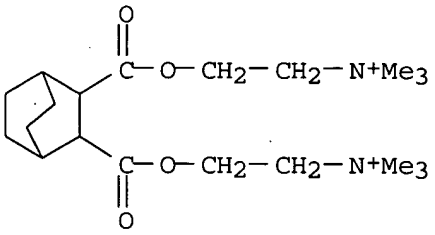
RN 7172-48-7 CAPLUS

CN Ammonium, ethyl(2-hydroxypropyl)dimethyl-, bromide, 5-norbornene-2,3-dicarboxylate, trans- (8CI) (CA INDEX NAME)



●2 Br^-

RN 10491-44-8 CAPLUS
CN Choline, iodide, bicyclo[2.2.2]octane-2,3-dicarboxylate, trans- (8CI) (CA INDEX NAME)



●2 I^-

L9 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1966:103735 CAPLUS
DOCUMENT NUMBER: 64:103735
ORIGINAL REFERENCE NO.: 64:19448h,19449a-e
TITLE: Basic esters of bicyclic diacids
PATENT ASSIGNEE(S): Firma F. Joh. Kwizda, Heinrich Koch, Johannes Kotlan
SOURCE: 7 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AT 244929		19660210	AT	19631211 <--

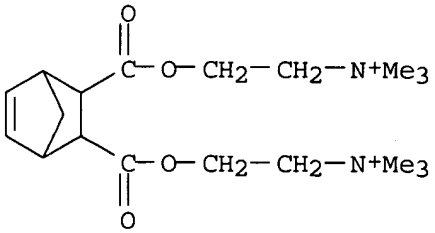
AB Bicyclic diacids (I) are esterified by basic alcs. to give II. The corresponding hydrogenated esters IV and the **quaternary** salts (II.R5X) (III) and (II.R5X) (V) of II and IV resp. are prepared All these compds. have pharmacol. properties, such as action on muscle nerves or blocking effect on ganglions. The esters are prepared from the dichlorides of I; e.g., a solution of 20 g. of dichloride of 1,4-endomethylene-2,3-trans-dicarboxy-5-cyclohexene (Ia) in 100 ml. benzene is added to 40 g. Me2NCH2CH2OH in 100 ml. benzene. The solution is refluxed, washed with 20% NaOH, and with water. Distillation gives II (n = 1, R1 = R2 = H, R4 = R3 = Me) in 95% yield, b2 180-90; n20D 1.4732; d254 1.0422. Corresponding III(n = 1) prepared are (R5X and m.p. given): HCl, 203-5°; MeI, 227-33°; EtI, 225-9°; EtBr, 191-5°. Hydrogenation of

the same II in AcOH over Pd-C gives IV (n = 1) in 80% yield: b2 175-80°; n25D 1.4729; d204 1.011. Corresponding V(n = 1) prepared are (R5X and m.p. given): HCl, 188-92°; MeI, 169-73°. Other aminoalcs. are used to give the following derivs.: II (n = 1, R3 = R4 = Et, R1 = R2 = H), b5 205-15°; n25D 1.4695; d204 0.9981; III (n = 1, R3 = R4 = Et, R1 = R = H (R5X and m.p. given): HCl, 149-53°; EtI, 247-53°; II (n = 1, R1 = H, R2 = R3 = R4 = Me), b5 190-5, n25D 1.4677, d204 1.0064; III (n = 1, R1 = H, R2 = R3 = R4 = Me), HCl, 228-32°; II[n = 1, R1 = R2 = H, (NR3R4) = piperidino], b5 205-25; n25D 1.4952; III [n = 1, R1 = R2 = H, NR3R4 = piperidino], HCl, deliquescent crystals; MeI, oil. In the 1,4-endoethylene-2,3-trans-dicarboxy-5-cyclohexene series (n = 2), the following compds. are prepared by the same method (R5X and mp. given): II (n = 2, R1 = R2 = H, R3 = R4 = Me), b2 175-95; III (n = 2, R1 = R2 = H, R3 = R4 = Me, R5X = MeI), m. 235-8°; II(n = 2, R1 = R2 = H, R3 = R4 = Et), b2 210-25; III (n = 2, R1 = R2 = H, R3 = R4 = Me), HCl, 163-8°; EtBr, 204-9°; II (n = 2, R3 = R4 = Me, R4 = H, R2 = Me), b2 200-10°; III (n = 2, R2 = R3 = R4 = Me, R1 = H), HCl, 170-80°; MeI, 215-30°. Transesterification is also used to prepare II. E.g., 20 g. of the di Me **ester** of 5,6:7,8-dibenzo-2,3-trans-dicarboxybicyclo[2.2.2]octane (Diels-Alder adduct between di-Me fumarate and anthracene) is added to a solution of 0.5 g. Na in 40 g. Me2NCH2CH2OH and heated on a water bath 5 hrs. The more volatile fraction is then removed by vacuum, and the residue dissolved in benzene and washed with water. After drying over Na2SO4 and evaporation of the solvent, the oily **ester** is purified by conversion into the corresponding dihydrochloride. Dimethiodide III (n = 1, R5X = HI) (IIIa) is prepared by another method: 22 g. of the dichloride of Ia are added to an excess of cold ethylene chlorhydrin. The rough dichloroethyl **ester** of Ia obtained is refluxed in 300 ml. acetone with 30 g. NaI. After elimination of NaCl and removal of the solvent, the bis(iodoethyl) **ester** of Ia is dissolved in ether and washed with water and thiosulfate solution The product is then heated in benzene solution with Me3N in a pressure bottle at 100° 6 hrs. IIIa is recrystd. from acetone-iso-PrOH.

IT **5561-81-9**, Choline, chloride, 5-norbornene-2,3-dicarboxylate, cis-
5783-18-6, Choline, iodide, 2,3-norbornanedicarboxylate, trans-
6012-28-8, 9,10-Ethanoanthracene-11,12-**dicarboxylic acid**, 9,10-dihydro-, diester with choline iodide, trans-
(preparation of)

RN 5561-81-9 CAPLUS

CN Choline, chloride, 5-norbornene-2,3-dicarboxylate, cis- (8CI) (CA INDEX NAME)

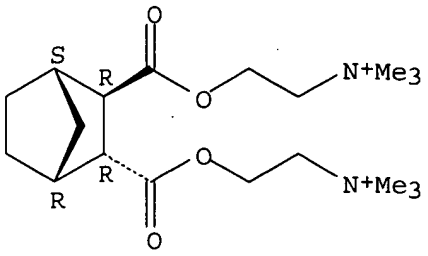


●2 Cl⁻

RN 5783-18-6 CAPLUS

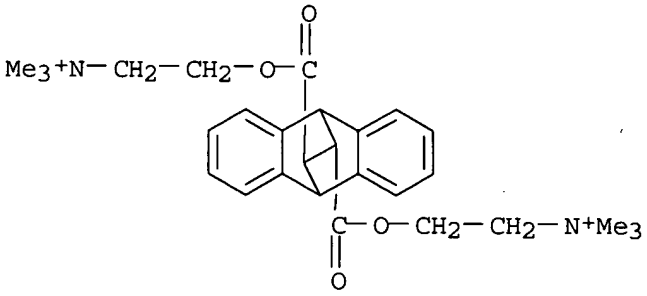
CN Ethanaminium, 2,2'-[bicyclo[2.2.1]heptane-2,3-diylbis(carbonyloxy)]bis[N,N,N-trimethyl-, diiodide, (2-endo,3-exo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



●2 I^-

RN 6012-28-8 CAPLUS
CN Ethanaminium, 2,2'-[(9,10-dihydro-9,10-ethanoanthracene-11,12-diyl)bis(carbonyloxy)bis[N,N,N-trimethyl-, diiodide, trans- (9CI) (CA INDEX NAME)



●2 I^-

L9 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1965:455342 CAPLUS
DOCUMENT NUMBER: 63:55342
ORIGINAL REFERENCE NO.: 63:10134a-c
TITLE: Plasticizer compositions
INVENTOR(S): Kay, Ronald W.
PATENT ASSIGNEE(S): Distillers Co. Ltd.
SOURCE: 5 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
FR 1391727		19650312	FR		<--
GB 1013605			GB		
NL 298427			NL		
PRIORITY APPLN. INFO.:			GB	19620929	

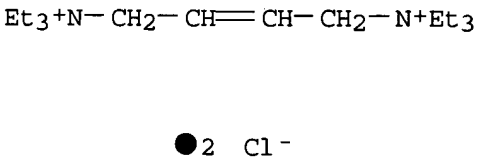
AB Alkali metal salts of an aromatic or aliphatic **dicarboxylic acid** monoester are heated with a mixture of 1,4-dichloro-2-butene (I) and a neutral alkali metal salt of an aromatic or aliphatic

dicarboxylic acid to give materials which can be used as plasticizers for poly(vinyl chloride) (II). Thus, 1.375 mole phthalic anhydride is dissolved in 1.52 mole BuOH at <105°, the solution is added in 1 hr. and 20 min. to a mixture of 1.25 mole I, 0.625 mole 1,4-C6H4(CO2Na)2, 0.757 mole Na2CO3, 0.016 mole Me3(PhCH2)NCl, and 312 ml. BuOH as the temperature rises from 116° to 123°, and the H2O-BuOH azeotrope is distilled The mixture is refluxed 10 hrs., washed with H2O, washed with NaOH, washed with H2O, and distilled to give 436 g. **ester** (III) saponification number 445. III (50 parts) is incorporated in 100 parts II to give a product, tensile strength 262.5 kg./cm.2, elongation at break 300%, melt index 19, volatilization loss 0.6%, as compared with 259, 280, 23, and 0.7, resp., for the control.

IT **3388-64-5**, Ammonium, 2-butene-1,4-diylbis[triethyl-, chloride (as catalyst in esterification of 1,4-dichloro-2-butene with monobutyl esters of phthalic or succinic acids alone or with phthalic or succinic acid alkali metal salts)

RN 3388-64-5 CAPLUS

CN Ammonium, 2-butene-1,4-diylbis[triethyl-, dichloride (8CI) (CA INDEX NAME)



2 Cl^-

L9 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1964:414046 CAPLUS

DOCUMENT NUMBER: 61:14046

ORIGINAL REFERENCE NO.: 61:2368g-h,2369a-b

TITLE: Chemical and pharmacological investigations in the series of cyclobutane **dicarboxylic acid** derivatives: curarelike activity of bisquaternary salts of basic esters or amides of α-, ε-, and γ-truxillic acids

AUTHOR(S): Arendaruk, A. P.; Kravchuk, L. A.; Skoldinov, A. P.; Kharkevich, D. A.

SOURCE: Uch. Zap., Inst. Farmakol. i Khimioterapii, Akad. Med. Nauk SSSR (**1963**), 3, 138-57

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

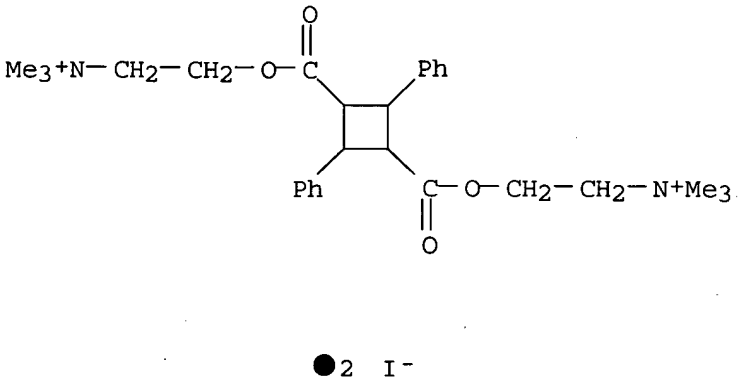
AB The curarelike activities of thesin (di-d-isoretronecanol **ester** of p,p'-dihydroxy-α-truxillic acid; CA 54, 24835cf) and its diiodomethylate (CA 55, 15366a) were the starting point for a closer investigation of structure-activity relations of a large number of bisquaternary salts of basic esters and amides of ε-(I), γ-(II), and α-truxillic (III) acids with the scope of elucidating the influence of (1) distance between cationic centers, (2) nature of substituents at the **quaternary** N atoms, and (3) structure of the chain between cationic centers. Determination of medium effective doses (E.D.50) was carried out on rabbits by the head-drop method; blocking of excitation transmission from the sciatic nerve to the gastrocnemius muscle was studied in decerebrate cats. The [XR(CH2)n]2 diiodide derivs. of III possessed greatest activity, where X = Et2N, piperidino, or 1-pyrrolidinyl, R = Me, and n = 3 and 4 (E.D.50, 25-33 γ/kg.; transmission blocking 100-150 γ/kg.). Compds. with n = 2, 5, 6, 7, or XMe2N, morpholino and R = Me, Et were less active, dimethiodides of dimethylaminoalkyl esters of III least active. The

influence of chain structure was studied in the dialkylaminopropylamides of I, II, and III, which possessed longer activity than the bisquaternary salts of the corresponding esters. Here also, activity decreased in the order III, I, and II derivs. All compds. investigated are nondepolarizing muscle relaxants. The X = piperidino, R = Et, n = 4 derivative, with E.D.50 = 41 γ/kg. was proposed for clin. investigation as truxillone.

IT **10066-71-4**, Choline, iodide, 2,4-diphenyl-1,3-cyclobutanedicarboxylate **17924-61-7**, 1,3-Cyclobutanedicarboxylic acid, diester with diethyl(2-hydroxyethyl)methylammonium iodide, cis- (preparation, chemistry and pharmacology of)

RN 10066-71-4 CAPLUS

CN Choline, iodide, 2,4-diphenyl-1,3-cyclobutanedicarboxylate (2:1), cis-1,2,trans-1,3,trans-1,4- (8CI) (CA INDEX NAME)

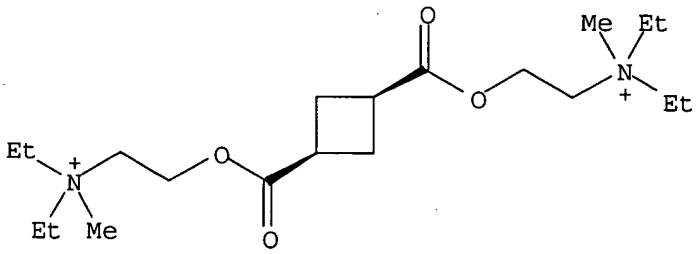


●2 I⁻

RN 17924-61-7 CAPLUS

CN Ammonium, diethyl(2-hydroxyethyl)methyl-, iodide, 1,3-cyclobutanedicarboxylate (2:1), cis- (8CI) (CA INDEX NAME)

Relative stereochemistry.



●2 I⁻

L9 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:	1961:124971 CAPLUS
DOCUMENT NUMBER:	55:124971
ORIGINAL REFERENCE NO.:	55:23573a-i,23574a-b
TITLE:	Muscarine. XI. Synthesis of bisquaternary compounds related to muscarine
AUTHOR(S):	Kiss, J.; Furter, H.; Lohse, F.; Hardegger, E.
CORPORATE SOURCE:	Eidg. Tech. Hochschule, Zurich, Switz.
SOURCE:	Helvetica Chimica Acta (**1961**), 44, 141-7 CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE:	Journal

LANGUAGE: German
OTHER SOURCE(S): CASREACT 55:124971

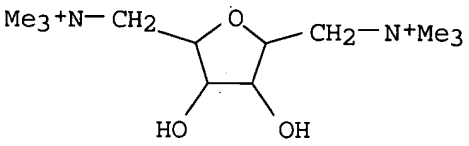
AB cf. CA 54, 601b. Five compds. related to muscarine were prepared from D-glucosamine-HCl (I) or L-glucosaminic acid (II). To a vibrated solution of 6 g. D-glucosaminic acid (III) in 36 ml. N HCl was added slowly during 3 hrs. at 0-5° 2.5 g. $NaNO_2$ in 40 ml. H_2O. After standing 20 hrs. at 20°, the solution was evaporated in vacuo at 40°, the alc. solution of the residue was filtered, evaporated, the residue in H_2O neutralized with excess $CaCO_3$, the solution again filtered and evaporated, the viscous oil was digested six times with 40 ml. Me_2CO, the residual Ca chitarate dissolved in 150 ml. H_2O, and by ion exchange (Nalcite HCR) converted into chitaric acid, m. 146°, contaminated by the lactone. This acid was dissolved in a 10-fold quantity of MeOH and treated 24 hrs. with excess Me_2NH at room temperature Evaporation in vacuo gave chitaric acid dimethylamide (IV), m. 172° (EtOAc), $[\alpha]D$ 18.8° (c 1, MeOH). IV (2.4 g.) in 11 ml. HNO_3 (d. 1.2) was carefully warmed to 65°. A vigorous reaction occurred, ending after 30-5 min. After repeated evapns. of the aqueous solns., the remaining viscous oil was crystallized from Me_2CO to yield 63% 2,5-anhydro-D-saccharic acid 1-dimethylamide (V), decomposing at 203-4°, $[\alpha]D$ -2.4° (c 2.5, H_2O). From the mother liquor 2,5-anhydro-D-saccharic acid (VI) was isolated via the Ca salt (yield 0.32 g.), m. 170-1° (Me_2CO-Et_2O), $[\alpha]D$ 39.3° (c 2, H_2O). Sublimation of V in high vacuum at 220° gave 2,5-furandicarboxylic acid (VII), decomposing at 300-20°. Oxidation of 15 g. I with 41 ml. HNO_2 (d. 1.2) at 60° gave via the Ca salt 19% crude 2,5-anhydro-D-manno-saccharic acid (VIII), m. 182° (alc.-Et_2O), $[\alpha]D$ 46.3° (c 1, H_2O). Esterification of VIII in MeOH with ethereal CH_2N_2 yielded quant. the di-Me **ester** hemihydrate (IX), m. 71° (MeOH-Et_2O), $[\alpha]D$ 45.3° (c 2.5, H_2O). IX (3.1 g.) in 10 ml. MeOH with 5 g. Me_2NH 2 hrs. at 65° in an autoclave yielded 2.2 g. VIII bis(dimethylamide) (X), m. 126° (EtOAc), $[\alpha]D$ 93.3° (c 1.5, H_2O). Esterification of V in MeOH with excess ethereal CH_2N_2 yielded V 6-Me **ester** (XI), m. 165-6° (EtOAc), $[\alpha]D$ 11.5° (c 1, H_2O). XI (0.4 g.) in 5 ml. cold MeOH treated with 5 g. Me_2NH in the cold and kept 24 hrs. at room temperature yielded 0.34 g. 2,5-anhydro-D-saccharic acid bis(dimethylamide) (XII), decomposing at 202° (MeOH), $[\alpha]D$ -52.2° (c 2, H_2O). XII was also prepared from 0.3 g. VI via the di-Me **ester**; yield 0.28 g. From 1.2 g. XI in 10 ml. MeOH, saturated with NH_3 at 0°, 0.91 g. 2,5-anhydro-D-saccharic acid 1-dimethylamide 6-**amide** was obtained, decomposing at 234°, $[\alpha]D$ 3.6° (c 3.5, H_2O). Treatment of 2.5 g. XII in 15 ml. dry pyridine with 0.9 g. tosyl chloride in 15 ml. pyridine 24 hrs. at room temperature and after warming to 35° addition of 40 ml. EtOAc yielded 170 mg. 3,4-ditosyl-2,5-anhydro-D-saccharic acid 1,6-bis(dimethylamide) (XIII), m. 202-3° ($CHCl_3$-EtOAc), $[\alpha]D$ 7.8° (c 0.65, $CHCl_3$). Ca salt of VII (5 g.) in 150 ml. H_2O was hydrogenated 6 hrs. with 5 g. Raney Ni at 150°/135 atmospheric in an autoclave. After removal of the Ca++ ions by ion exchange (Nalcite HCR), 55% cis-tetrahydrofuran-2,5-**dicarboxylic acid** (XIV) was obtained, m. 125-6° (EtOAc-petr. ether). XIV was converted into its di-Me **ester** (XV) by the diazomethane method. Treatment of 1.02 g. XV in 10 ml. MeOH with 2 g. Me_2NH 2 hrs. at 90° gave 920 mg. XIV bis(dimethylamide) (XVI). The bis(dimethylamides) X, XII, XIII, and XVI were reduced by slow addition of these compds. in dioxane to $LiAlH_4$ in dioxane, the excess $LiAlH_4$ decomposed by EtOAc, the solution evaporated, 50 ml. 10N NaOH/g. $LiAlH_4$ added, the tertiary amines repeatedly extracted with Et_2O, and after evaporation **quaternized** by boiling in excess MeI. Thus, 1.5 g. X in 80 ml. dioxane gave after 3 hrs. reflux, etc., 1.26 g. 1,6-dideoxy-1,6-bis(dimethylamino)-2,5-anhydro-D-mannitol-2MeI, decomposing at 299-300° (80% alc.), $[\alpha]D$ 32.2° (c 1, H_2O). XII (0.5

g.) gave 510 mg. 1,6-dideoxy-1,6-bis(dimethylamino)-2,5-anhydro-D-sorbitol-2MeI (XVII), decomposing at 300° (75% alc.), [α]D 13.6° (c 1, H2O). Reduction of XIII gave two products because of partial or total reductive cleavage of the tosyl groups. Thus, 114 mg. XIII in 30 ml. dioxane with 200 mg. LiAlH4 in 40 ml. dioxane gave after 2 hrs. at 80-90° and 1 hr. reflux 68 mg. crude methiodide. The fraction, difficultly soluble in alc., gave after several recrystns. from 80% alc. 3- or 4-deoxy analog of XVII, decomposing at 298-300° [α]D 2.8° (c 0.7, H2O). The fraction, well soluble in alc., gave 18 mg. cis-2,5-bis(dimethylaminomethyl)tetrahydrofuran-2MeI (XVIII), decomposing at 302° (alc.), showing no rotation. The structure of XVIII was confirmed by the isolation of an identical product from the reduction of XVI in the above way. The L-form of XVII was prepared in exactly the same way as described for XVII, starting from II, with corresponding values of the phys. consts.

IT **88777-26-8**, Sorbitol, 2,5-anhydro-1,6-dideoxy-1,6-bis(dimethylamino)-, dimethiodide **109215-30-7**, Mannitol, 2,5-anhydro-1,6-dideoxy-1,6-bis(dimethylamino)-, dimethiodide
(preparation of)

RN 88777-26-8 CAPLUS

CN D-Glucitol, 2,5-anhydro-1,6-dideoxy-1,6-bis(trimethylammonio)-, diiodide (9CI) (CA INDEX NAME)

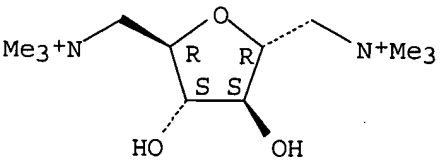


●2 I-

RN 109215-30-7 CAPLUS

CN Mannitol, 2,5-anhydro-1,6-dideoxy-1,6-bis(dimethylamino)-, dimethiodide (6CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 I-

L9 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1959:94742 CAPLUS

DOCUMENT NUMBER: 53:94742

ORIGINAL REFERENCE NO.: 53:17092f-i,17093a-g

TITLE: Pyrroles. XIV. Mannich bases of 2,5-substituted pyrroles

AUTHOR(S): Herz, Werner; Settine, Robert L.

CORPORATE SOURCE: Florida State Univ., Tallahassee

SOURCE: Journal of Organic Chemistry (**1959**), 24,

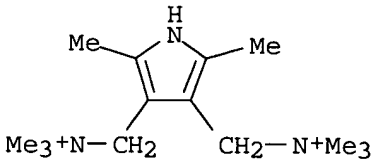
201-4
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C.A. 53, 7136h. Several pyrroles substituted in the 2-and 5-positions of the pyrrole nucleus were subjected to the Mannich reaction. The resulting bases were shown to be 3-dialkylaminomethyl- and 3,4-bis(dialkylaminomethyl) derivs. of pyrrole. Their utility as alkylating agents was investigated. The following general procedures were used for the preparation of the Mannich bases, Me2NCH2C:CR.NR'CR: CH (I) and Me2NCH2C: CR.NR'CR:CCH2NMe2 (II). Method A. NHMe2.HCl (85 g.)in 79 g. 40% HCHO added at 60° to 100 g. 2,5-dimethylpyrrole, diluted with H2O, extracted with Et2O, and the aqueous layer poured into 200 ml. 25% NaOH gave 148 g. product. For disubstitution, the quantities of NHMe2.HCl and HCHO were doubled. Method B. NHMe2 (20 ml., 33%) and 20 ml. AcOH mixed with 8.5 ml. 40% HCHO, and the solution added dropwise under N to 17.1 g. 1-phenyl-2,5-dimethylpyrrole gave 11.1 g. product. For disubstitution, 2 moles aqueous NHMe2 and 2 moles HCHO were used. The picrates were precipitated by mixing alc. solns. of the base and picric acid and recrystg. from alc. Methiodides were prepared by addition of I or II, dissolved in a min. of alc., to 10% excess MeI with stirring at ice bath temperature and recrystg. from alc. (type of compound, R, R', % yield, m.p. or b.p./mm., method, m.p. of MeI derivative, and m.p. of picrate given): I, Me, H, 92, 99-100°, A, 130° (decomposition), 117-18°; I, Me, Ph, 49.5, 130-1°/1, B, 211-12° (decomposition), 137-8°; I, Me, Me, 69, 73-4°/1, B, 140° (decomposition), 137-8° (decomposition); I, Ph, H, 73, 124-5% B, -, 179-80°; II, Me, H, 90, 144-5°, A, 139-40°, 139-40°; II, Me, Ph, 61, 150°/1, B, 100° (decomposition), 200-1° (decomposition); II, Me, Me, 72.5, 96-7°/0.3, B, -, 181-2° (decomposition). II (R = Me, R' = H) (20 g.) in 100 ml. alc. heated 48 hrs. at 100° with 4 g. Raney Ni and H at 80-100 atmospheric gave 7.7 g. 2,3,4,5-tetramethylpyrrole, m. 107-8°, by steam distillation In a similar manner hydrogenolysis of 20 g. I (R = Me, R' = H) 8 hrs. at 80-90° gave 1.5 g. 2,3,5-trimethylpyrrole, b15 79-80°, and 7.5 g. of starting material. Di-Et acetamidomalonate (III) (16.2 g.) and 11.5 g. I (R = Me, R' = H) mixed with 100 ml. alc. containing 1.72 g. Na, treated dropwise at 35° with 15.8 g. Me2SO4, stirred overnight, and concentrated gave 18.4 g. di-Et 2,5-dimethyl-3-pyrrolylmethyl-α-acetamidomalonate (IV), m. 176-7° (alc.-H2O). Reaction of 26 g. I with 32.4 g. III in 300 ml. PhMe containing 1 g. powdered NaOH gave 24 g. IV. Condensation of 20.3 g. di-Et formamidomalonate (IVa) and 11.5 g. I (R = Me, R' = H) in alc. by **quaternization** in situ gave 19.2 g. di-Et 2,5-dimethyl-3-pyrrolylmethyl-α-formamidomalonate (V), m. 137-8.5°. Hydrolyzing 6 g. V with 50 ml. 25% NaOH 2.5 hrs., cooling, acidifying, filtering, acidifying the filtrate to pH 5, and seeding gave 3.3 g. crude material which was chromatographed to show one spot; the analysis indicated the presence of inorg. material which could not be removed. CH2(CO2Et)2 (VI) (50 g.) with 31.5 g. I (R = Me, R' = H) by **quaternization** gave 35.5 g. di-Et 2,5-dimethyl-3-pyrrolylmethylmalonate, b2 173-5°. Reaction of 20.8 g. 2,5-diphenyl-3-(dimethylaminomethyl)pyrrole and 20.3 g. IVa by the in situ **quaternization** method gave 31.05 g. di-Et 2,5-diphenyl-3-pyrrolylmethyl-α-formamidomalonate (VII), m. 164-5° (alc.-H2O). VII (5 g.), 10 g. KOH, and 50 ml. 80% alc. refluxed overnight gave 1.5 g. 2,5-diphenyl-3-pyrrolealanine, m. 217-18° (decomposition). VI (64 g.) containing 1.84 g. Na heated 6 hrs. at 120° under N with 26 g. I.MeI (R = Me, R' = Ph), H2O added, and the mixture extracted with Et2O and distilled gave 23.6 g. VI and 11.4 g. di-Et 1-phenyl-2,5-dimethyl-3-

pyrrolylmethylmalonate, b0.1 164-5°, n25D 1.5230. By the above procedure there was obtained after 24 hrs. 6.8 g. di-Et 1,2,5-trimethyl-3-pyrrolylmethylmalonate, b0.9 145-6°, n25D 1.4670. I.MeI (R = Me, R' = Me) (55 g.), 30 g. NaCN, and 200 ml. H2O heated under N until evolution of basic gas ceased gave 5.5 g. 1,2,5-trimethyl-3-pyrroleacetonitrile (VIII), b0.2 90°, n25D 1.1527, ν 2250 cm.-1. The pot residue consisted of a tarry solid which liberated NH3 on treatment with base and probably contained some **amide**, due to partial hydrolysis of VIII. VIII (5 g.), 5 g. KOH, and 50 ml. 80% alc. refluxed 8 hrs., diluted with H2O, and poured over ice containing 10 ml. concentrated HCl, and the oil which separated taken up in Et2O gave 3.2 g. 1,2,5-trimethyl-3-pyrroleacetic acid (IX), m. 120-1° (ligroine). 1,2,5-Trimethylpyrrole (90 g.) and 4 g. Cu powder treated dropwise with 48 g. N2CHCO2Et, stirred 3 hrs., the Cu removed, and the filtrate distilled in vacuo gave 72.5 g. unchanged pyrrole and 18.8 g. Et 1,2,5-trimethyl-3-pyrroleacetate (X), b5 124-5°, n27D 1.4919. Hydrolysis of X with 80% alc. alkali gave 2.76 g. IX. I.MeI (R = Me, R' = Ph) (40 g.) and 30 g. NaCN similarly gave 9 g. 1-phenyl-2,5-dimethyl-3-pyrroleacetonitrile (XI), b0.6 144-5°, n25D 1.5246, ν 2250 cm.-1 (CN band). XI (3 g.) on saponification gave 2.5 g. 1-phenyl-2,5-dimethyl-3-pyrroleacetic acid, m. 151-2° (ligroine).

IT **109286-53-5**, Ammonium, [(2,5-dimethylpyrrole-3,4-diyl)dimethylene]bis[trimethyl- iodide]
(preparation of)

RN 109286-53-5 CAPLUS

CN [(2,5-Dimethylpyrrole-3,4-diyl)dimethylene]bis[trimethylammonium iodide] (6CI) (CA INDEX NAME)



L9 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1959:94484 CAPLUS

DOCUMENT NUMBER: 53:94484

ORIGINAL REFERENCE NO.: 53:16994b-i,16995a-f

TITLE: Synthesis of some conjugated cyclobutane polyolefins and their 1,2-cycloaddition to tetracyanoethylene

AUTHOR(S): Blomquist, A. T.; Meinwald, Yvonne C.

CORPORATE SOURCE: Cornell Univ., Ithaca, NY

SOURCE: Journal of the American Chemical Society (**1959**), 81, 667-72
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 53:94484

AB 3-Methylene-1,4-diphenyl-2-methylcyclobutene (I) and diphenyldimethylenecyclobutene (II) were synthesized from β-truxinic acid (III) by a series of conventional transformations which included Hofmann degradation of appropriate bis(**quaternary** hydroxides) in the final steps. I and II reacted with (NC)2C:C(CN)2 (IV) by 1,2-cycloaddn. to yield spirocyclobutane derivs. 3-Methylenecyclohexene

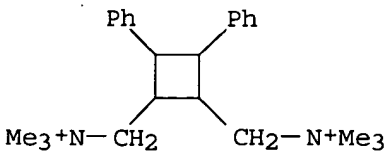
(V) showed similar 1,2-cycloaddn. IV and norbornadiene (VI) also formed a 1:1 adduct. III (64 g.), 300 cc. absolute EtOH, 150 cc. PhMe, and 3 cc. concentrated H_2SO_4 refluxed azeotropically and distilled gave 71.9 g. di-Et **ester** (VII) of III, m. 51°. VII (67.7 g.) in 100 cc. dry Et_2O reduced with 14.8 g. $LiAlH_4$ in 750 cc. dry Et_2O yielded 47.5 g. 1,2-bis(hydroxymethyl)-3,4-diphenylcyclobutane (VIII), m. 110-11° (MeOH). VIII (13.4 g.) added in several portions with stirring and cooling to 13.7 g. PBr_3, stirred at room temperature to solution, heated 8 hrs. at 80°, cooled, diluted with 25 cc. H_2O, extracted with C_6H_6, the extract washed, dried, evaporated, and the residue recrystd. from CCl_4-pentane yielded 15.2 g. 1,2-bis(bromomethyl)-3,4-diphenylcyclobutane (IX), 95.5-6.5°. IX (3.94 g.), 4.8 g. Me_3N, and 2 cc. MeOH kept 1 week at room temperature in a sealed tube gave 5 g. 1,2-bis(dimethylaminomethyl)-3,4-diphenylcyclobutane dimethobromide (X), characterized as the dipicrate, m. 255-6° (decomposition) (EtOH). X (2.56 g.) in 10 cc. H_2O treated with Ag_2O from 3.4 g. $AgNO_3$ and 1.4 g. KOH, stirred 2 hrs., filtered, evaporated, the residual glassy solid heated at 120-40°/0.4-0.5 mm., and the sublimate (0.75-0.9 g.) resublimed at 55°/0.4 mm. and recrystd. from MeOH gave I, needles, m. 63-4°. I in EtOAc hydrogenated at 25°/736.5 mm. over prereduced PtO_2 during 1 hr. and the crude product chromatographed on Al_2O_3 gave 2,3-diphenyl-1,4-dimethylcyclobutene, $n^{25}D$ 1.5892. I (114.3 mg.) in 30 cc. CH_2Cl_2 treated with ozonized O at -78° during 0.5 hr., added with stirring to 0.2 g. Zn dust in 10 cc. AcOH, stirred 0.5 hr. at room temperature, distilled into 200 mg. dimedon, a drop piperidine, and 10 cc. 75% EtOH, and the distillate heated until all CH_2Cl_2 was removed and cooled gave 35 mg. dimedon derivative of CH_2O, needles, m. 190-1°. IX (3.94 g.), 1.78 g. N-bromosuccinimide, a few crystals of Bz_2O_2, and 100 cc. CCl_4 refluxed 1 hr. and filtered, the filtrate concentrated to about 10 cc., and diluted with pentane gave 3.4 g. 3-Br derivative (XI) of IX, plates, m. 105-5.5° (decomposition). XI and excess Me_3N heated 2 days at 50° in MeOH in a sealed tube and the mixture evaporated gave 4.5 g. mixture of the 2(or 3)-butene analog (XII) and the 3(or 2)-analog (XIII) of X; the mixture extracted with CH_2Cl_2 left 1.5 g. of one of the isomers, m. 200-4° [picrate m. 228-30° (decomposition) (EtOH)]; the extract evaporated and the residue recrystd. from H_2O yielded the other isomer, m. 185-7°, which did not yield a solid picrate. Mixture (2.04 g.) of XII and XIII converted in the usual manner to the base mixture and the crude product (1.21 g.) pyrolyzed gave 0.28-0.35 g. crude product which resublimed at 40°/0.3 mm. gave II, m. 42-3°; II could be kept several days at 0° under N without visible change but it turned yellow at room temperature within a few hrs.; in all pyrolyses 0.25-0.3 g. dark polymeric residue was formed; it could be repptd. from C_6H_6 with hexane. II hydrogenated over PtO_2 absorbed 90% of 3 equivs. H. The reductive ozonolysis of II yielded 34% CH_2O. II (0.32 g.) in 2 cc. CCl_4 titrated at 0° with 10% Br in CCl_4 and evaporated in vacuo gave 0.75 g. 1,2-dibromo-1,2-bis(bromomethyl)-3,4-diphenyl-3-cyclobutene, m. 118-19° (Et_2O). II did not react at 25° with maleic anhydride, N-phenylmalimide, and (.tplbond.CCO_2Et)2 (XIV), but polymerization occurred in all cases at higher temps.; II and XIV heated at 150° and the crude product chromatographed gave a small amount of amorphous product, decompose 160-70°. II (0.34 g.), in a few cc. C_6H_6 treated under N with 0.35 g. IV in C_6H_6, refluxed 0.5 hr., kept at room temperature overnight, evaporated in vacuo, the dark residue extracted with boiling Et_2O to leave an insol. polymeric residue, and the extract treated with Norite and evaporated gave 0.18 g. 1,1,2,2-tetracyano-5,6-diphenyl-7-methylenespiro[3.3]-5-heptene (XV), needles, m. 175-6° (decomposition). XV (47 mg.) in 0.5 cc. $CHCl_3$ titrated with Br in $CHCl_3$, the solution evaporated,

and the crude residue recrystd. from Et2O gave 1,1,2,2-tetracyano-5-bromo-5-(bromomethyl)-6,7-diphenylspiro[3.3]-6-heptene, m. 162.5-63° (decomposition). I (0.2144 g.) in 5 cc. dry Et2O added to 0.120 g. IV in 10 cc. Et2O, shaken 3 hrs. at room temperature, and evaporated in vacuo gave 1,1,2,2-tetracyano-5,7-diphenyl-5-methylspiro[3.3]-5-heptene, light yellow glass, m. 139.5-40.5° (decomposition) (Et2O-petr. ether). Crude 2-cyclohexenemethanol (XVI) (13 g.) and 17.3 g. phthalic anhydride in 15 cc. PhMe refluxed 3 hrs., kept at room temperature overnight, diluted with Et2O, filtered, the filtrate extracted with aqueous Na2CO3, the alkaline extract acidified and extracted with CH2Cl2, the extract filtered and evaporated, and the residue recrystd. from hexane-Et2O gave acid phthalate (XVII) of XVI, m. 73.5-5.5° (hexane-Et2O). XVII (32 g.) in 180 cc. 25% aqueous NaOH refluxed 2 hrs. gave 12.7 g. pure XVI, b8 95°, n25D 1.4820, which treated with Ac2O and C5H5N at room temperature gave 16.7 g. acetate (XVIII) of XVI, b15 95-6°, n25D 1.4575. XVIII pyrolyzed at 525 ± 15° gave 6.9 g. crude pyrolyzate which fractionated gave V, b. 109-10°, n25D 1.4895. V (1.6 g.) added to 1.6 g. IV in C6H6, refluxed 10 min., kept at room temperature overnight, filtered, the filtrate evaporated, and the residue recrystd. from Et2O yielded 1.4 g. 1,1,2,2-tetracyanospiro[3.5]-5-nonene, m. 121-2° (decomposition) with softening and yellowing at 100-16° depending on the rate of heating. IV in C6H6 treated with the usual fashion with VI and the mixture refluxed 0.5 hr. yielded 100% 8,8,9,9-tetracyanoquadricyclo[2.2.1.02,6.23,5]nonane (XIX), m. 186-8° (decomposition) (C6H6); when the addition was carried out at room temperature during 3-4 days a lower melting form, m. 158-60°, of XIX was obtained in 100% yield; the lower melting form changed after standing at room temperature for more than 1 week to the higher melting modification. XIX (1.3 g.) refluxed 24 hrs. with 10 g. NaOH in 12 cc. H2O and 30 cc. EtOH, acidified, concentrated, diluted with 10 cc. H2O, extracted with Et2O, and the glassy residue (1.6 g.) recrystd. from C6H6-Et2O yielded 1.25 g. 8,9-dicarboxyquadricyclo[2.2.1.02,6.23,5]nonane-8,9-dicarboximide, m. 205-7° (with effervescence). Methylene-1,2-cyclopropanedicarboxylic acid, methylenecyclobutane, methylenecyclononane, and norbornene added to saturated solns. of IV in C6H6, kept at room temperature overnight, and heated several hrs. at 80-90° gave only unchanged starting materials. The infrared absorption spectra of I and II are recorded.

IT **121447-16-3**, Ammonium, [(3,4-diphenyl-1,2-cyclobutylene)dimethylene]bis[trimethyl-] **122568-22-3**, Ammonium, [[3,4-diphenyl-3-cyclobuten-1,2-ylene]dimethylene]bis[trimethyl-] **122568-24-5**, Ammonium, [[3,4-diphenyl-2-cyclobuten-1,2-ylene]dimethylene]bis[trimethyl-]
(-salts)

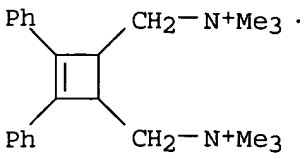
RN 121447-16-3 CAPLUS

CN 1,2-Cyclobutanedimethanaminium, N,N,N,N',N',N'-hexamethyl-3,4-diphenyl- (9CI) (CA INDEX NAME)

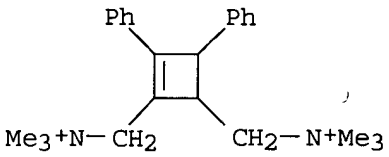


RN 122568-22-3 CAPLUS

CN 3-Cyclobutene-1,2-dimethanaminium, N,N,N,N',N',N'-hexamethyl-3,4-diphenyl- (9CI) (CA INDEX NAME)



RN 122568-24-5 CAPLUS
CN 2-Cyclobutene-1,2-dimethanaminium, N,N,N,N',N',N'-hexamethyl-3,4-diphenyl- (9CI) (CA INDEX NAME)

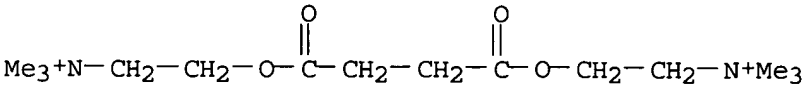


L9 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1959:72288 CAPLUS
DOCUMENT NUMBER: 53:72288
ORIGINAL REFERENCE NO.: 53:13065b-d
TITLE: Curare-like **quaternary** salts of basic esters of aliphatic dicarboxylic acids
INVENTOR(S): Wunderlich, Helmut
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 11654		19560602	DD	<--

AB Bis-ω-haloalkylesters (I) of aliphatic dicarboxylic acids (II) are treated with gaseous Me3N in an inert solvent (e.g., Et2O, Me2CO, C6H6) to give **quaternary** salts. I and II are prepared from dihalides (preferably dibromides) of the acids with ethylene oxide. The **dicarboxylic acid** dichlorides may be converted into the dibromides by heating with gaseous HBr. E.g., 310 g. succinyl dichloride is brominated with HBr at 45° until the weight is 500-20 g., then fractionated to yield 85-90% succinyl dibromide III, b12 108-14°. III (488 g.) and a few crystals ZnCl2 is treated with 200 g. ethylene oxide and fractionated to give 85-90% succinylbis(bromoethyl) **ester**, b3.5 163-70° (IV). IV (166 g.) is dissolved in 400 cc. dry Me2CO and treated with a minute excess of Me3N gas yielding crystalline succinylbischoline **ester** dibromide, m. 225-7°, yield 80-5% (MeOH).

IT **55-94-7**, Choline, bromide succinate
(preparation of)
RN 55-94-7 CAPLUS
CN Ethanaminium, 2,2'-[(1,4-dioxo-1,4-butanediyl)bis(oxy)]bis[N,N,N-trimethyl-, dibromide (9CI) (CA INDEX NAME)



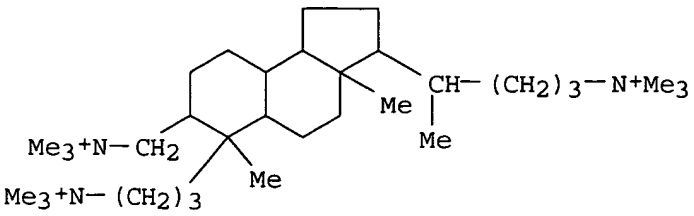
●2 Br^-

L9 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1958:50718 CAPLUS
DOCUMENT NUMBER: 52:50718
ORIGINAL REFERENCE NO.: 52:9173i,9174a-c
TITLE: Multivalent **quaternary** ammonium compounds. VI. Some reaction products of bile acids and sterols
AUTHOR(S): Lettre, H.; Gottstein, W.; Scholtissek, Ch.
CORPORATE SOURCE: Univ. Heidelberg, Germany
SOURCE: Monatshefte fuer Chemie (**1957**), 88, 715-20
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 51, 4409a. Some N derivs. of lithiobilianic acid (I) and sitosterol are prepared I is treated with Ac2O followed by Me2NH to yield lithiobilianic acid 3-monodimethylamide, m. 251-2°. I with Ac2O followed by PCl5 and then with Me2NH in Et2O gives an Et2O phase containing 60%-70% I 3,4,24-tris(dimethylamide), m. 151-2°, purified by chromatography on Al2O3. The aqueous phase of the reaction yields 15-20% of I 3,24-bis(dimethylamide) (II), m. 232-3°. II is esterified with CH2N2 and reduced with LiAlH4 in tetrahydrofuran to 3,4-secocholan-4-ol-3,24-bis(dimethylamine hydrochloride), m. 292-5° (decomposition). II is similarly reduced to 90% 3,4-secocholane-3,4,24-tris(dimethylamine hydrochloride), decompose 275°, which forms 3,4-secocholane-3,24-tris(trimethylammonium iodide), m. 290° (decomposition). The **dicarboxylic acid** of sitosterol (III), heated 2 hrs. with Ac2O gives 76% 2,3-secositostanol-2,3-**dicarboxylic acid** anhydride, m. 176°. III di-Me **ester** is reduced by LiAlH4 to 88% 2,3-secositostane-2,3-diol, m. 182-3° (MeOH). III with PCl5 and Me2NH yields by chromatography on Al2O3 48% 2,3-secositostane-2,3-**dicarboxylic acid** dimethylamide, m. 106-7°, reduced by LiAlH4 to 68% 2,3-secositostane-2,3-bis(dimethylamine hydrochloride), m. 326° (decomposition). This compound with MeI gives 2,3-secositostane-2,3-bis(trimethylammonium iodide), m. 323°.

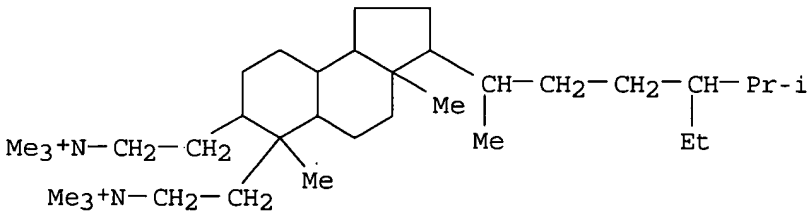
IT **122387-46-6**, 3,4-Secocholane-3,4,24-triamine, N3,N3,N4,N4,N24,N24-hexamethyl-, trimethiodide **125496-38-0**, 2,3-Secositostane-2,3-diamine, N2,N2,N3,N3-tetramethyl-, dimethiodide
(preparation of)

RN 122387-46-6 CAPLUS
CN 3,4-Secocholane-3,4,24-triamine, N3,N3,N4,N4,N24,N24-hexamethyl-, trimethiodide (6CI) (CA INDEX NAME)



●3 I⁻

RN 125496-38-0 CAPLUS
CN 2,3-Secositostane-2,3-diamine, N2,N2,N3,N3-tetramethyl-, dimethiodide (6CI) (CA INDEX NAME)



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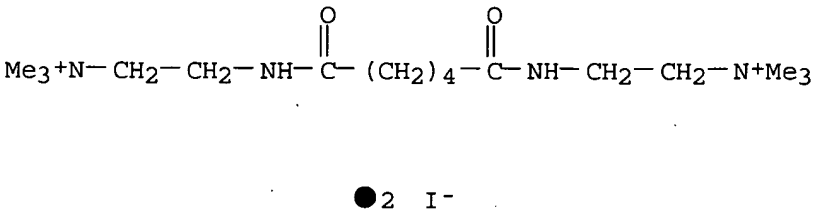
L9 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1953:70520 CAPLUS
DOCUMENT NUMBER: 47:70520
ORIGINAL REFERENCE NO.: 47:11905a-c
TITLE: Bolaform electrolytes. III. Conductance of bisquaternary salts of **dicarboxylic acid** bis-2-tertiary-aminoalkyl amides in methanol
AUTHOR(S): Eisenberg, H.; Fuoss, Raymond M.
CORPORATE SOURCE: Yale Univ.
SOURCE: Journal of the American Chemical Society (**1953**), 75, 2914-17
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C.A. 45, 6017e. The conds. in MeOH at 25° of the following salts were measured: N,N'-bis(2-dimethylaminoethyl)oxalamide-di-MeI, N,N'-bis(2-dimethylaminoethyl)succinamide-di-MeI, N,N'-bis(2-dimethylaminoethyl)adipamide-di-MeI, and N,N'-bis(2-dimethylaminoethyl)suberamide-di-MeI. These salts are bolaform electrolytes with, resp., 8, 10, 12, and 14 atoms joining their 2 **quaternary** nitrogens. The constant k2, which describes the interaction of a bolaform cation and an anion, is practically the same for the oxalic and the suberic derivs., and is somewhat larger for these compds. than for the succinic and adipic derivs. This observation suggests that an intramol. ring structure, stabilized by H bonds between the **amide** groups is formed, which shortens the effective charge-charge distance.
IT **62055-16-7**, Ammonium, [adipoylbis(iminoethylene)]bis[trimethyl-

iodide]
(elec. conductivity in MeOH, and structure of)
RN 62055-16-7 CAPLUS
CN Ethanaminium, 2,2'-[(1,6-dioxo-1,6-hexanediyl)diimino]bis[N,N,N-trimethyl-, diiodide (9CI) (CA INDEX NAME)



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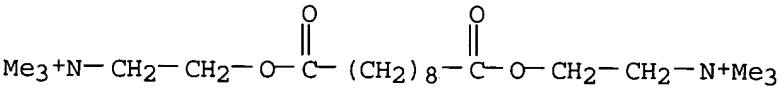
L9 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1952:3443 CAPLUS
DOCUMENT NUMBER: 46:3443
ORIGINAL REFERENCE NO.: 46:626d-e
TITLE: The pharmacology of α,ω-bisquarternary ammonium compounds. III. Comparison of several **dicarboxylic acid** esters
AUTHOR(S): Ginzel, K. H.; Klupp, H.; Werner, G.
CORPORATE SOURCE: Univ. Vienna
SOURCE: Archives Internationales de Pharmacodynamie et de Therapie (**1951**), 87, 79-98
CODEN: AIPTAK; ISSN: 0003-9780
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The neuromuscular blocking action in nonanesthetized dogs and chloralosed cats and the spastic paralysis in pigeons decrease with increasing C-chain length of the following: bischoline esters of succinic, adipic, and sebacic acids and their ethyl derivs. The contracture response of the isolated rectus abdominis of the frog increased with chain length and was antagonized by d-tubocurarine. The hypertensive effect also increased in this manner. However, the adipic acid diester of triethyl(2-hydroxyethyl)ammonium iodide caused flaccid paralysis in pigeons and reduced the sensitivity of the frog rectus abdominis to acetylcholine.
IT **17140-07-7**, Sebacic acid, **ester** with choline iodide
(pharmacology of)
RN 17140-07-7 CAPLUS
CN Ethanaminium, 2,2'-[(1,10-dioxo-1,10-decanediyl)bis(oxy)]bis[N,N,N-trimethyl-, diiodide (9CI) (CA INDEX NAME)



2 I-

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L2          50 S L1

     FILE 'CAPLUS' ENTERED AT 11:19:32 ON 27 JUN 2005
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               S L1

     FILE 'REGISTRY' ENTERED AT 11:20:12 ON 27 JUN 2005
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     FILE 'CAPLUS' ENTERED AT 11:20:13 ON 27 JUN 2005
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L6       10617 S L5 AND PY<1999
L7         927 S L6  AND (ESTER OR AMIDE)
L8         316 S L7 AND QUATERN?
L9          17 S L8 AND DICARBOXYLIC ACID
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               S L1

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     FILE 'CAPLUS' ENTERED AT 11:29:24 ON 27 JUN 2005
L12          3 S L11
               S L10

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L13       2365 S L10 FULL

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L14       1441 S L13 FULL
L15       1111 S L14 AND PY<1999
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L17         43 S L16 AND QUATERN?
L18          1 S L17 AND DICARBOXYLIC ACID

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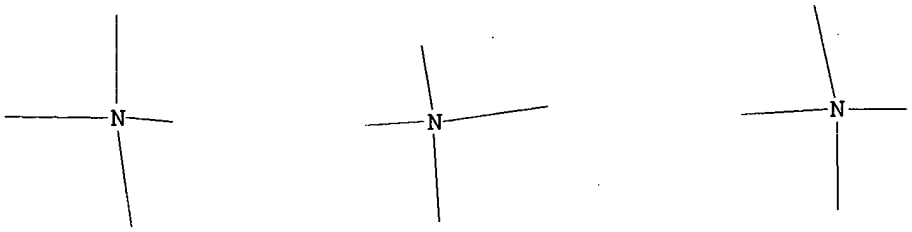

Structure attributes must be viewed using STN Express query preparation.

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76.4% PROCESSED 1000 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
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PROJECTED ANSWERS: 21103 TO 25183

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L12 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:182792 CAPLUS
DOCUMENT NUMBER: 142:263559
TITLE: Preparation of shamrock surfactants and their methods of use
INVENTOR(S): Jaeger, David A.
PATENT ASSIGNEE(S): University of Wyoming, USA
SOURCE: PCT Int. Appl., 46 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2005019405 A1 20050303 WO 2003-US29742 20030922

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-495214P P 20030813

AB Shamrock surfactants are surfactants containing two ionic or polar nonionic head groups, each connected to a central ionic head group by a hydrocarbon linking moiety, wherein the central head group is a dithiophosphate, dithiocarbamate, or quaternary ammonium group. These surfactants have potential applications in chemical decontamination of mustard (simulants), storage and release devices/chemical switches and the remediation of heavy-metal ion-contaminated water. Such a surfactant compound is of the formula [X-L-Z-L'-X'](A)p, wherein X and X' represent outer head groups, which may be the same or different and comprise charged moieties selected from the group of -N+R1R2R3, R1, R2 and R3 being the same or different, representing hydrocarbyl groups, -CO2- or -O(CH2)mSO3-, m being an integer from 2 to 30, or polar moieties of the formula, -O-(CH2CH2O)nR4, R4 being hydrogen or a C1-C6 hydrocarbyl group and n is an integer from 1 to 1000; L and L' are the same or different and represent a hydrocarbon linking moiety which may optionally be interrupted with oxygen; Z represents a central head group selected from a dithiophosphate moiety, dithiocarbamate or a quaternary ammonium moiety, wherein R5 and R6 are the same or different and represent C1-C6 hydrocarbyl groups, with the proviso that when Z represents said dithiocarbamate moiety or said quaternary ammonium moiety, X and X' do not represent N+R1R2R3, and with the further proviso that X and X' do not represent -O(CH2)mSO3- unless Z represents said quaternary ammonium moiety; and A represents a counter ion, which may be either pos. or neg. depending on the net charge of [X-L-Z-L'-X'] and p is an integer which, when multiplied by the valency of said counter ion yields the absolute value of the net charge of [X-L- Z-L'-X'].

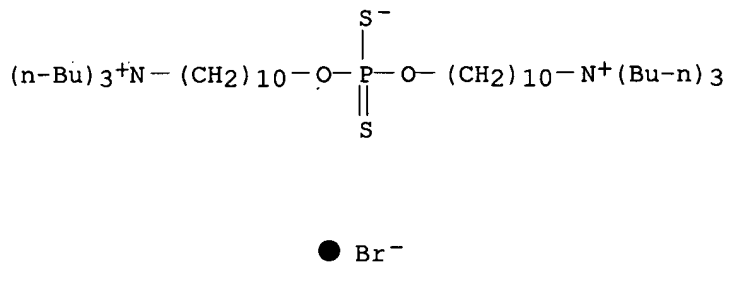
IT **813446-48-9P**

RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of shamrock surfactants and their methods of use)

RN 813446-48-9 CAPLUS

CN 16,18-Dioxa-5-azonia-17-phosphaoctacosan-28-aminium, N,N,N,5,5-pentabutyl-17-mercapto-, inner salt, bromide, 17-sulfide (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

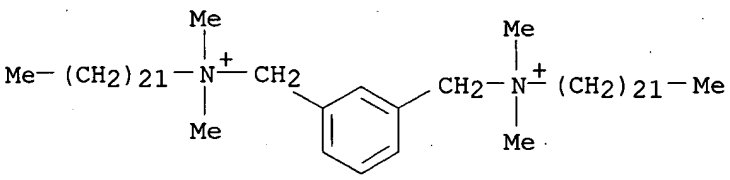
ACCESSION NUMBER: 2004:1030565 CAPLUS

DOCUMENT NUMBER: 142:446807
TITLE: Promotion effect of cationic Gemini surfactants on 1-dodecene hydroformylation in biphasic catalytic system
AUTHOR(S): Xu, Bin; Li, Min; Yang, Min; Zheng, Hong-Jie; He, Yu-E.; Chen, Hua; Li, Xian-Jun
CORPORATE SOURCE: Institute of Homogeneous catalysis, College of Chemistry, Sichuan University, Chengdu, 610064, Peop. Rep. China
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (2004), 25(11), 2060-2064
CODEN: KTHPDM; ISSN: 0251-0790
PUBLISHER: Gaodeng Jiaoyu Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB New cationic Gemini surfactants with a rigid spacer group of xylene were synthesized, their compns. and structures were characterized. The cmc and the solubilizations of 1-dodecene in micellar solution were determined by surface tension method and UV-Vis spectrometry resp. The cmc of new Gemini surfactants are lower than CTAB by about an order, but the solubilizations of 1-dodecene in Gemini surfactants solution are higher than that in CTAB solution The promotion effect of cationic Gemini surfactants on 1-dodecene hydroformylation in biphasic catalytic system was studied. The results indicated that in the biphasic system containing the catalysts RhCl(CO)(TPPTS)2 and TPPTS, [TPPTS = tris (sodium-m-sulfonatophenyl) phosphine], the reaction rate of 1-dodecene hydroformylation in the presence of Gemini surfactants was faster than that in the presence of conventional surfactant CATB, e.g., the conversion of 1-dodecene is 90% when G (o-xyl)c22 concentration in aqueous solution was 2 + 10-3 mol/L, however, the conversion was only 20.4% when the concentration of CTAB was 3 + 10-3 mol/L. The greater acceleration of Gemini surfactants in 1-dodecene hydroformylation could be attributed to that cationic Gemini surfactants had lower cmc and better solubilization for the substrate. The lower cmc arid surface tension are favorable for increasing the interfacial area of two phases, breaking phase barrier and promoting the substrate transfer to interface where the substrates coordinate with the active rhodium complex anion species. The regioselectivity for olefin hydroformylation in Gemini surfactants.

IT **851319-26-1**
RL: NUU (Other use, unclassified); PRP (Properties); RGT (Reagent); RACT (Reactant or reagent); USES (Uses)
(promotion effect of cationic Gemini surfactants on 1-dodecene hydroformylation in biphasic catalytic system)

RN 851319-26-1 CAPLUS
CN 1,3-Benzenedimethanaminium, N,N'-didocosyl-N,N,N',N'-tetramethyl-, dibromide (9CI) (CA INDEX NAME)



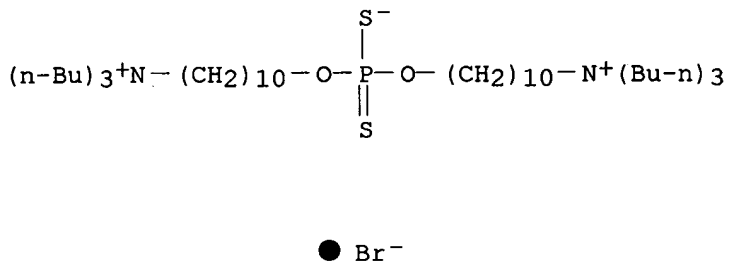
●2 Br⁻

L12 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:902647 CAPLUS
DOCUMENT NUMBER: 142:76557
TITLE: Shamrock Surfactants: Synthesis and Characterization
AUTHOR(S): Jaeger, David A.; Zeng, Xiaohui; Apkarian, Robert P.
CORPORATE SOURCE: Department of Chemistry, University of Wyoming, Laramie, WY, 82071, USA
SOURCE: Langmuir (2004), 20(24), 10427-10432
CODEN: LANGD5; ISSN: 0743-7463
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two types of a new class of surfactants with 3 headgroups were prepared A central headgroup is connected to 2 flanking headgroups by hydrocarbon chains. The term "shamrock" is used to describe these surfactants, denoting their triple-headed character and reflecting the fact that shamrocks have leaflets in groups of 3. The major lipophilic character of shamrock surfactants is provided by the 2 hydrocarbon chains linking the 3 headgroups and not by long-chain alkyl groups appended to the linking hydrocarbon chains or the headgroups. The new surfactants are (2,2,15,15,28,28-hexamethyl-2,15,28-triazonianonacosane triiodide), (2,2,15,15,28,28-hexamethyl-2,15,28-triazonianonacosane trichloride) (I), (O,O'-di-[10-(N,N,N-tripropylammonio)decyl]phosphorodithioate bromide), and (O,O'-di-[10-(N,N,N-tributylammonio)decyl]phosphorodithioate bromide). (2,2,9,9,16,16-Hexamethyl-2,9,16-triazoniaheptadecane triiodide) was prepared for comparison. The surfactants were characterized in water by measurement of their Krafft temps. and critical aggregation concns., and their aggregates were studied by 1H NMR spectroscopy, dynamic laser light scattering, and phase-contrast optical microscopy. Aqueous I was also studied by cryo-etch high-resolution SEM, which revealed irregularly shaped cells containing a complex matrix of surfactant. Coacervates were observed by optical microscopy upon the hydration of the shamrock surfactants.

IT **813446-48-9P**
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(synthesis and characterization of trilobal shamrock surfactants)

RN 813446-48-9 CAPLUS
CN 16,18-Dioxa-5-azonia-17-phosphaoctacosan-28-aminium, N,N,N,5,5-pentabutyl-17-mercapto-, inner salt, bromide, 17-sulfide (9CI) (CA INDEX NAME)



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

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SEARCH TIME: 00.00.01

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L15        1111 L14 AND PY<1999

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L17          43 L16 AND QUATERN?

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        3995178 ACID
          36503 DICARBOXYLIC ACID
                (DICARBOXYLIC(W)ACID)
L18           1 L17 AND DICARBOXYLIC ACID

=> d ibib abs hitstr

L18  ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         1958:50718  CAPLUS
DOCUMENT NUMBER:          52:50718
ORIGINAL REFERENCE NO.:   52:9173i,9174a-c
TITLE:                    Multivalent quaternary ammonium compounds.
                          VI. Some reaction products of bile acids and sterols
AUTHOR(S):                Lettre, H.; Gottstein, W.; Scholtissek, Ch.
CORPORATE SOURCE:         Univ. Heidelberg, Germany
SOURCE:                   Monatshefte fuer Chemie (1957), 88, 715-20
                          CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE:            Journal
LANGUAGE:                 Unavailable
AB   cf. C.A. 51, 4409a.  Some N derivs. of lithiobilianic acid (I) and
     sitosterol are prepared  I is treated with Ac2O followed by Me2NH to yield
     lithiobilianic acid 3-monodimethylamide, m. 251-2°.  I with Ac2O
     followed by PCl5 and then with Me2NH in Et2O gives an Et2O phase containing
     60%-70% I 3,4,24-tris(dimethylamide), m. 151-2°, purified by
     chromatography on Al2O3.  The aqueous phase of the reaction yields 15-20% of I
     3,24-bis(dimethylamide) (II), m. 232-3°.  II is esterified with
     CH2N2 and reduced with LiAlH4 in tetrahydrofuran to 3,4-secocholan-4-ol-
     3,24-bis(dimethylamine hydrochloride), m. 292-5° (decomposition).  II is
     similarly reduced to 90% 3,4-secocholane-3,4,24-tris(dimethylamine
     hydrochloride), decompose 275°, which forms 3,4-secocholane-3,24-
```
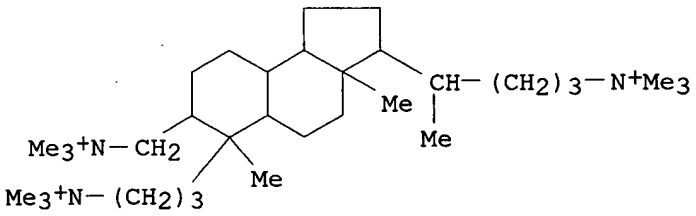

tris(trimethylammonium iodide), m. 290° (decomposition). The **dicarboxylic acid** of sitosterol (III), heated 2 hrs. with Ac2O gives 76% 2,3-secositostanol-2,3-**dicarboxylic acid** anhydride, m. 176°. III di-Me **ester** is reduced by LiAlH4 to 88% 2,3-secositostane-2,3-diol, m. 182-3° (MeOH). III with PCl5 and Me2NH yields by chromatography on Al2O3 48% 2,3-secositostane-2,3-**dicarboxylic acid** dimethylamide, m. 106-7°, reduced by LiAlH4 to 68% 2,3-secositostane-2,3-bis(dimethylamine hydrochloride), m. 326° (decomposition). This compound with MeI gives 2,3-secositostane-2,3-bis(trimethylammonium iodide), m. 323°.

IT **122387-46-6**, 3,4-Secocholane-3,4,24-triamine, N3,N3,N4,N4,N24,N24-hexamethyl-, trimethiodide
(preparation of)

RN 122387-46-6 CAPLUS

CN 3,4-Secocholane-3,4,24-triamine, N3,N3,N4,N4,N24,N24-hexamethyl-, trimethiodide (6CI) (CA INDEX NAME)



●3 I⁻

=> d l17 1-10 ibib abs hitstr

L17 ANSWER 1 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:737708 CAPLUS
DOCUMENT NUMBER: 137:237406
TITLE: A **quaternary** ammonium phosphate-containing aqueous composition suitable for the application to human skin
INVENTOR(S): Zeigler, Philip Dale; Cheney, Michael Charles
PATENT ASSIGNEE(S): Hindustan Lever Ltd., India
SOURCE: Indian, 40 pp.
CODEN: INXXAP
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IN 173884	A	19940730	IN 1992-BO5691	19920220 <--
PRIORITY APPLN. INFO.:			IN 1992-BO5691	19920220

OTHER SOURCE(S): MARPAT 137:237406

AB An aqueous composition is provided which includes a **quaternary** ammonium functionalized phosphate **ester** and a cationic polysaccharide. The compns. may include an emollient, and be used as a water-proof sunscreen composition For example, a sunscreen composition was prepared from (by

weight): Phase A containing cetyl alc. 2.5%, glycerol monostearate (Kessco GMS) 1.5%, Pr paraben 0.10%, ethylhexyl p-methoxycinnamate (Parsol MCX) 7.0%, oxybenzone (Uvinul M-40) 3.0%, octyl palmitate (Schercemol OP) 2.0%, silicone fluid 1.0%, and petroleum jelly 1.0%, and Phase B containing glycerin 4.0%, Monaquat P-TS 3.0%, Antifoam AF 0.005%, Me paraben 0.150%, Quatrisoft LM-200 0.250%, fragrance 0.150%, and water up to 100%.

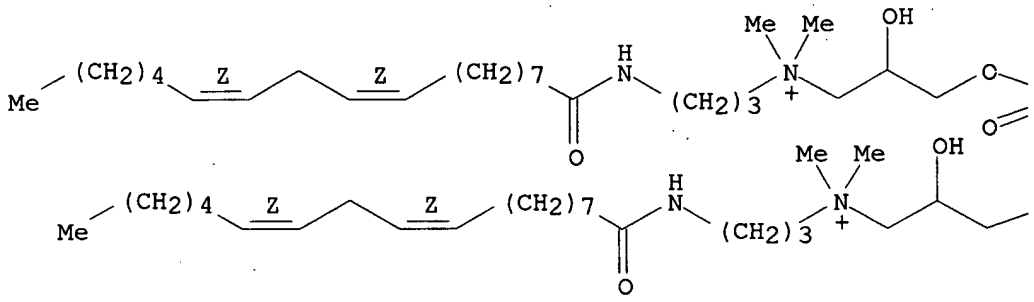
IT **144377-73-1**, Phospholipid EFA **144379-29-3**, Monaquat P-TS
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(cosmetic compns. containing **quaternary** ammonium phosphate and cationic polysaccharide)

RN 144377-73-1 CAPLUS

CN 4,6-Dioxa-14-aza-10-azonia-5-phosphadotriaconta-23,26-dien-1-aminium, 5-[3-[dimethyl[3-[[(9Z,12Z)-1-oxo-9,12-octadecadienyl]amino]propyl]ammonio]-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-15-oxo-N-[3-[[(9Z,12Z)-1-oxo-9,12-octadecadienyl]amino]propyl]-, trichloride, 5-oxide, (23Z,26Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



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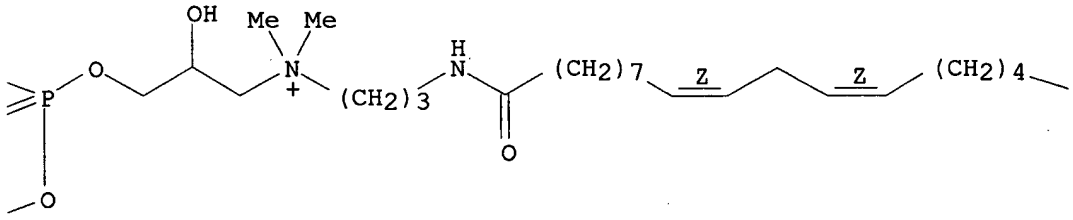
PAGE 1-B



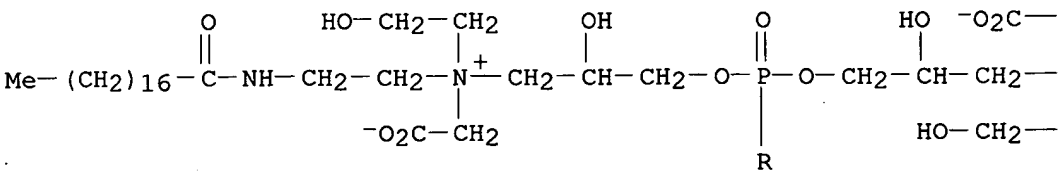
PAGE 1-C

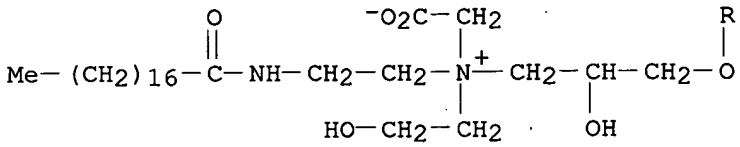
RN 144379-29-3 CAPLUS

CN 4,6-Dioxa-13-aza-10-azonia-5-phosphahentriacontan-1-aminium,

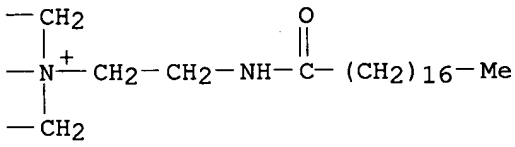
N,10-bis(carboxymethyl)-5-[3-[(carboxymethyl)(2-hydroxyethyl)[2-[(1-oxooctadecyl)amino]ethyl]ammonio]-2-hydroxypropoxy]-2,8-dihydroxy-N,10-bis(2-hydroxyethyl)-14-oxo-N-[2-[(1-oxooctadecyl)amino]ethyl]-, tris(inner salt), 5-oxide (9CI) (CA INDEX NAME)

PAGE 1-A





PAGE 1-B



L17 ANSWER 2 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:766507 CAPLUS
DOCUMENT NUMBER: 130:29221
TITLE: Preparation of solid porous matrixes for pharmaceutical uses
INVENTOR(S): Unger, Evan C.
PATENT ASSIGNEE(S): ImaRx Pharmaceutical Corp., USA
SOURCE: PCT Int. Appl., 139 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9851282	A1	19981119	WO 1998-US9570		19980512 <--
W: AU, BR, CA, CN, JP, KR, NZ					
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE					
US 2002039594	A1	20020404	US 1998-75477		19980511
AU 9873787	A1	19981208	AU 1998-73787		19980512 <--
EP 983060	A1	20000308	EP 1998-921109		19980512
R: DE, FR, GB, IT, NL					
US 2001018072	A1	20010830	US 2001-828762		20010409
US 2004091541	A1	20040513	US 2003-622027		20030716
PRIORITY APPLN. INFO.:			US 1997-46379P	P	19970513
			US 1998-75477	A	19980511

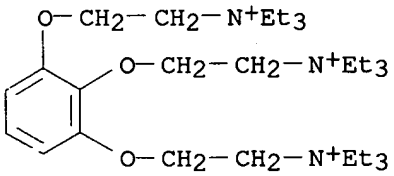
WO 1998-US9570 W 19980512
US 2001-828762 B1 20010409

AB A solid porous matrix formed from a surfactant, a solvent, and a bioactive agent is described. Thus, amphotericin nanoparticles were prepared by using ZrO2 beads and a surfactant. The mixture was milled for 24 h.

IT **65-29-2**, Gallamine triethiodide
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of solid porous matrixes for pharmaceutical uses)

RN 65-29-2 CAPLUS

CN Ethanaminium, 2,2',2''-[1,2,3-benzenetriyltris(oxy)]tris[N,N,N-triethyl-, triiodide (9CI) (CA INDEX NAME)



●3 I⁻

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 3 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:648717 CAPLUS
DOCUMENT NUMBER: 127:333127
TITLE: Softening agents containing polycationic surfactants for fabrics in laundering
INVENTOR(S): Imada, Hiroshi; Imai, Hiroto; Sugafuji, Hisahiro; Fujiwara, Masami
PATENT ASSIGNEE(S): Lion Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09256273	A2	19970930	JP 1996-67691	19960325 <--
PRIORITY APPLN. INFO.:			JP 1996-67691	19960325

OTHER SOURCE(S): MARPAT 127:333127

AB The agents, used during the rinse cycle, which soften fabrics without affecting hydrophilicity and yellowing prevention, contain polycationic surfactants R3(R1R4N+A)nN+R2R5R6 (n + 1)X-, cationic surfactants R7(N+R8R9G)mN+R10R11R12 (m + 1)X-, and anionic surfactants R13CH(SO3X1)CO2R14 (A = C2-12 alkylene, hydroxyalkylene; G = C2-10 alkylene; R1, R2, R7 = C10-28 saturated hydrophobic group; R3-R6, R8-R12 = C1-6 alkyl, hydroxyalkyl; R13 = C8-26 alkyl; R14 = C1-6 alkyl; X = halogen; X1 = H, metal, ammonium; m ≥ 0; n ≥ 1). Thus, reacting 2 mol N,N-dimethylstearylamine and 1 mol 1,6-diiodohexane to give a diquaternary ammonium salt (I), sep. reacting 1 mol Duomeen HT Flake, 4 mol HCHO, and excess HCO2H, followed by reaction with MeCl to give another **quaternary** ammonium salt (II), mixing I 0.9, II 0.1, and Na Me α-sulfostearate 0.5 equiv, and dissolving the mixture in water at 3%

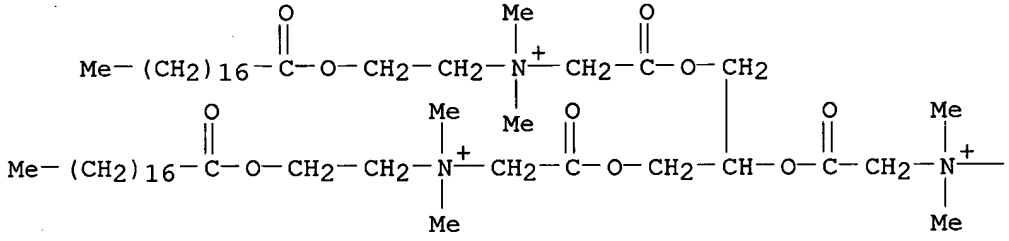
gave a softening agent. A cotton towel was washed and rinsed in a washing machine; then the agent was added at 0.0033%. After the towel was squeezed and dried, it showed good softness and good water absorbency.

IT **197862-15-0P**
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(polycationic; softening agents containing polycationic surfactants, cationic surfactants, and anionic surfactants for fabrics after laundering)

RN 197862-15-0 CAPLUS

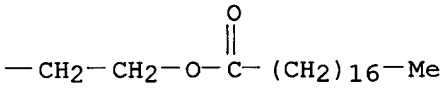
CN 3,7,13-Trioxa-10-azoniahentriacontan-1-aminium, 5-[[[dimethyl[2-[(1-oxooctadecyl)oxy]ethyl]ammonio]acetyl]oxy]-N,N,10,10-tetramethyl-2,8,14-trioxo-N-[2-[(1-oxooctadecyl)oxy]ethyl]-, trichloride (9CI) (CA INDEX NAME)

PAGE 1-A



●3 Cl⁻

PAGE 1-B



L17 ANSWER 4 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:369695 CAPLUS
DOCUMENT NUMBER: 126:347155
TITLE: Cosmetic compositions containing cationic resin and waxes
INVENTOR(S): Sheard, Christine
PATENT ASSIGNEE(S): Boots Company Plc, UK; Sheard, Christine
SOURCE: PCT Int. Appl., 21 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9713497	A1	19970417	WO 1996-EP4393	19961009 <--
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE,				

ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS,
LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD,
SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR,
IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA

AU 9672893	A1	19970430	AU 1996-72893		19961009 <--
EP 862410	A1	19980909	EP 1996-934606		19961009 <--
EP 862410	B1	20021218			
R: DE, FR, GB					
ZA 9608552	A	19980610	ZA 1996-8552		19961010 <--
PRIORITY APPLN. INFO.:			GB 1995-20690	A	19951010
			WO 1996-EP4393	W	19961009

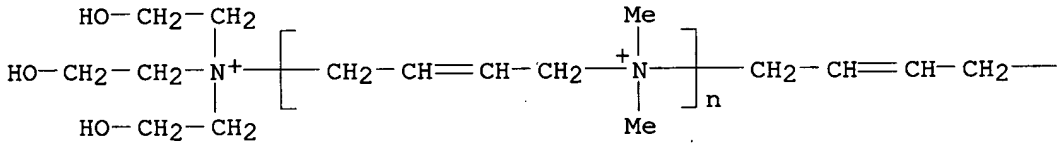
AB A cosmetic composition comprises 0.05-5% hydrophilic cationic resin 30-85% oil component 1-40% wax component and 1-40 % weight/weight powder component. The hydrophilic cationic resin may be water soluble or water swellable and may also be any mixture of suitable homopolymers or copolymers, e.g., any mixture of 1 or more Polyquaternium polymers or polymeric salts preferably those denoted by the CFTA name Polyquaternium. The cosmetic composition is solid at ambient temperature and is suitable for use as a lipstick. A product comprising the composition associated with a suitable receptacle and/or dispenser is also disclosed. Thus, a lipstick contained plant wax 6.4, paraffin wax 9.0, synthetic wax 2.3, synthetic fat 10.0, fatty alc. 20.7, synthetic **ester** 12.74, plant oil 26.24, preservative 0.1, antioxidant 0.03, Salcare SC96 2.25, butylene glycol 1.5, and pigment 8.74%.

IT **75345-27-6**, Polyquaternium-1
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(cosmetic compns. containing cationic resin and waxes)

RN 75345-27-6 CAPLUS

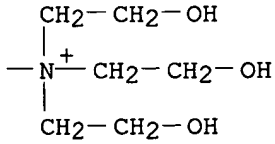
CN Poly[(dimethyliminio)-2-butene-1,4-diyl chloride], α-[4-[tris(2-hydroxyethyl)ammonio]-2-butenyl]-ω-[tris(2-hydroxyethyl)ammonio]-, dichloride (9CI) (CA INDEX NAME)

PAGE 1-A



●3 Cl⁻

PAGE 1-B



L17 ANSWER 5 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:329281 CAPLUS
DOCUMENT NUMBER: 126:308638

TITLE: Body wash compositions containing anionic cleansing surfactants polymeric cationic conditioning compounds and **quaternized** phosphate esters

INVENTOR(S): Scafidi, Anthony A.
PATENT ASSIGNEE(S): Helene Curtis, Inc., USA

SOURCE: PCT Int. Appl., 59 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9710804	A1	19970327	WO 1996-US14410	19960909 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI				
US 5683683	A	19971104	US 1995-531712	19950921 <--
ZA 9607294	A	19970304	ZA 1996-7294	19960828 <--
CA 2231809	AA	19970327	CA 1996-2231809	19960909 <--
AU 9669697	A1	19970409	AU 1996-69697	19960909 <--
BR 9610522	A	19990706	BR 1996-10522	19960909
PRIORITY APPLN. INFO.:			US 1995-531712 A	19950921
			WO 1996-US14410 W	19960909

OTHER SOURCE(S): MARPAT 126:308638

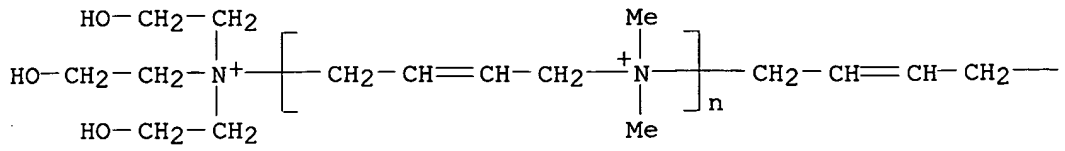
AB A body wash composition containing an anionic cleansing surfactant, such as an alkyl ether sulfate or an alkyl sulfate, like sodium lauryl ether sulfate or sodium lauryl sulfate; a polymeric cationic conditioning compound, such as a **quaternized** guar gum; and a **quaternized** phosphate **ester** in an aqueous carrier is disclosed. The composition is used to cleanse and to impart conditioning properties to the skin. A body wash composition contained sodium lauryl ether sulfate 12.0, a premixed surfactant concentrate 3.6 , cocamide MEA 7.0, preservatives 0.5, guar hydroxypropyltrimonium chloride 0.2, tetrasodium ethylenediamine tetraacetic acid 0.08, citric acid 0.15, palmitic acid 2.0, stearamidopropyl phosphatidyl PG-dimonium chloride 0.4, cocamidopropyl hydroxysultate 1.9, titanium dioxide 0.2, and water q.s. 100%.

IT **75345-27-6**, Polyquaternium 1
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(body wash compns. containing anionic cleansing surfactants polymeric cationic conditioning compds. and **quaternized** phosphate esters)

RN 75345-27-6 CAPLUS

CN Poly[(dimethyliminio)-2-butene-1,4-diyl chloride], α-[4-[tris(2-hydroxyethyl)ammonio]-2-butenyl]-ω-[tris(2-hydroxyethyl)ammonio]-, dichloride (9CI) (CA INDEX NAME)

PAGE 1-A



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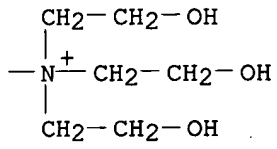


L17 ANSWER 6 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:656984 CAPLUS
DOCUMENT NUMBER: 125:308699
TITLE: Emulsified, low pH cosmetic compositions having improved stability
INVENTOR(S): Papadakis, Marcelline C.
PATENT ASSIGNEE(S): Helene Curtis, Inc., USA
SOURCE: U.S., 10 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5567427	A	19961022	US 1995-406106	19950317 <--
WO 9629051	A1	19960926	WO 1996-US3761	19960314 <--
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML				
AU 9653175	A1	19961008	AU 1996-53175	19960314 <--
PRIORITY APPLN. INFO.:			US 1995-406106 A	19950317
			WO 1996-US3761 W	19960314

AB Emulsified, low pH cosmetic compns. having improved pH and phase stability are disclosed. The emulsified cosmetic compns. have a pH 3.7-4.5, and contain 10-50% by weight dispersed oil phase, 2-20% by weight acid, like a hydroxycarboxylic acid, and 0.5-2% **quaternized** phosphate **ester**, like linoleamidopropyl PG-dimonium chloride phosphate. The emulsified cosmetic compns. are phase-stable over an extended storage period and maintain a constant pH by exhibiting a pH drift of about 0.15, usually ≤0.1 pH units.

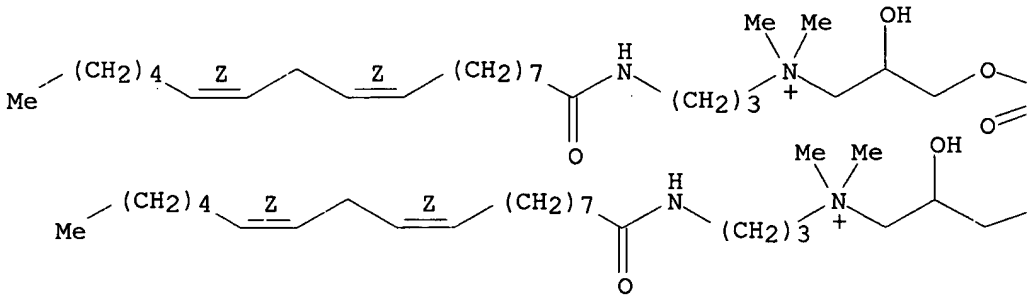
IT **144377-73-1**, Phospholipid EFA
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(emulsified, stable, low pH cosmetic compns. containing)

RN 144377-73-1 CAPLUS

CN 4,6-Dioxa-14-aza-10-azonia-5-phosphadotriaconta-23,26-dien-1-aminium, 5-[3-[dimethyl[3-[[(9Z,12Z)-1-oxo-9,12-octadecadienyl]amino]propyl]ammonio]-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-15-oxo-N-[3-[[(9Z,12Z)-1-oxo-9,12-octadecadienyl]amino]propyl]-, trichloride, 5-oxide, (23Z,26Z)- (9CI) (CA INDEX NAME)

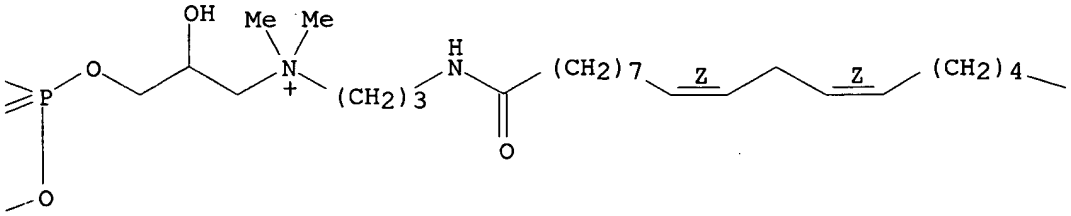
Double bond geometry as shown.

PAGE 1-A



●3 Cl⁻

PAGE 1-B



PAGE 1-C

L17 ANSWER 7 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:	1996:377496 CAPLUS
DOCUMENT NUMBER:	125:118113
TITLE:	Automatic dishwashing detergent compositions comprising multiquaternary bleach activators
INVENTOR(S):	Sivik, Mark R.; Taylor, Lucille F.; Burckett St.Laurent, James C. T.
PATENT ASSIGNEE(S):	The Procter and Gamble Company, USA
SOURCE:	U.S., 20 pp., Cont.-in-part of U.S. Ser. No. 298,904. CODEN: USXXAM
DOCUMENT TYPE:	Patent
LANGUAGE:	English

FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5520835	A	19960528	US 1995-438126	19950508 <--
US 5578136	A	19961126	US 1994-298904	19940831 <--
US 5654421	A	19970805	US 1995-486654	19950607 <--
CA 2154704	AA	19960301	CA 1995-2154704	19950726 <--
CA 2154704	C	19990615		
CA 2244021	AA	19960301	CA 1995-2244021	19950726 <--
CA 2244021	C	20021119		
ES 2202342	T3	20040401	ES 1995-305458	19950804
EP 742280	A2	19961113	EP 1996-302491	19960409 <--
EP 742280	A3	19991201		
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
CA 2175275	AA	19961109	CA 1996-2175275	19960429 <--
CA 2175275	C	19990831		

PRIORITY APPLN. INFO.: US 1994-298904 A2 19940831
US 1995-438126 A 19950508

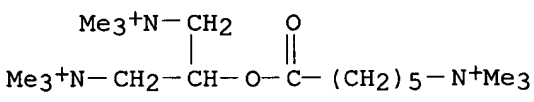
OTHER SOURCE(S): MARPAT 125:118113

AB The title compns., especially granular detergents, comprise bleach activators (structures specified) containing multiple **quaternary** N groups, preferably ≥3 such groups and preferably have ≥1 **quaternary** N group in the peracid-forming portion of the bleach activator as well as ≥1 **quaternary** N group in the leaving-group portion. Thus, H2N(CH2)5CO2H·HCl obtained by hydrolysis of ε-caprolactam with HCl was N-methylated with HCHO/HCO2H, the product was acid chlorinated with COCl2, then esterified with HOCH(CH2NMe2)2 and the **ester quaternized** with MeCl to give the title activator 3-[Me3N+(CH2)5CO2]CH(CH2N+Me3)2·3H Cl.

IT **179325-36-1DP**, salts with compatible anions **179325-37-2P** **179325-38-3P** **179325-39-4DP**, salts with compatible anions **179325-40-7DP**, salts with compatible anions **179325-41-8DP**
, salts with compatible anions
RL: IMF (Industrial manufacture); PREP (Preparation)
(automatic dishwashing detergent compns. comprising multiquaternary bleach activators)

RN 179325-36-1 CAPLUS

CN 1,3-Propanediaminium, N,N,N,N',N',N'-hexamethyl-2-[[1-oxo-6-(trimethylammonio)hexyl]oxy]- (9CI) (CA INDEX NAME)

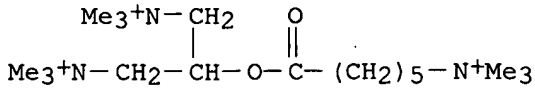


RN 179325-37-2 CAPLUS

CN 1,3-Propanediaminium, N,N,N,N',N',N'-hexamethyl-2-[[1-oxo-6-(trimethylammonio)hexyl]oxy]-, tris(methyl sulfate) (9CI) (CA INDEX NAME)

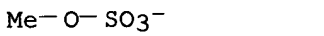
CM 1

CRN 179325-36-1
CMF C18 H42 N3 O2

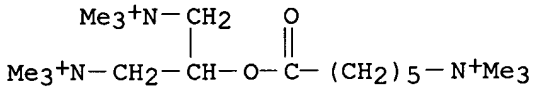


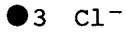
CM 2

CRN 21228-90-0
CMF C H3 O4 S

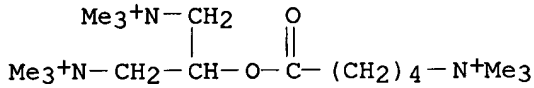


RN 179325-38-3 CAPLUS
CN 1,3-Propanediaminium, N,N,N,N',N',N'-hexamethyl-2-[[1-oxo-6-(trimethylammonio)hexyl]oxy]-, trichloride (9CI) (CA INDEX NAME)

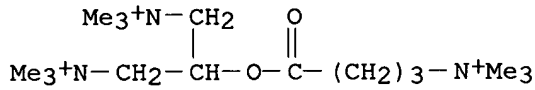




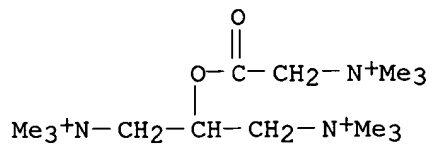
RN 179325-39-4 CAPLUS
CN 1,3-Propanediaminium, N,N,N,N',N',N'-hexamethyl-2-[[1-oxo-5-(trimethylammonio)pentyl]oxy]- (9CI) (CA INDEX NAME)



RN 179325-40-7 CAPLUS
CN 1,3-Propanediaminium, N,N,N,N',N',N'-hexamethyl-2-[1-oxo-4-(trimethylammonio)butoxy]- (9CI) (CA INDEX NAME)



RN 179325-41-8 CAPLUS
CN 1,3-Propanediaminium, N,N,N,N',N',N'-hexamethyl-2-[[(trimethylammonio)acetyl]oxy]- (9CI) (CA INDEX NAME)



L17 ANSWER 8 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:153898 CAPLUS
DOCUMENT NUMBER: 124:264081
TITLE: Liquid bleaching compositions for textiles with good

storage stability

INVENTOR(S): Ogura, Nobuyuki; Ozaki, Kazuyoshi; Hishige, Takaomi; Aoyanagi, Muneo

PATENT ASSIGNEE(S): Kao Corp, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07331289	A2	19951219	JP 1994-129113	19940610 <--
JP 3330226	B2	20020930		

PRIORITY APPLN. INFO.: JP 1994-129113 19940610

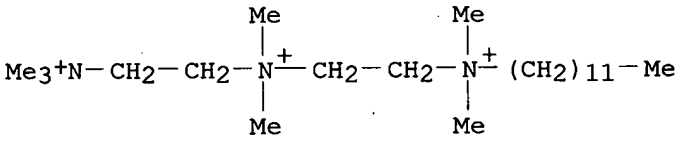
OTHER SOURCE(S): MARPAT 124:264081

AB The bleaching compns. contain H2O2, bleaching activators which form organic acids on reaction with H2O2, polycationic compds. R1R2R3N+(R4N+R5R6)nR7.(n + 1)Z- [R1,R2, R3, R5, R6, and/or R7 is C8-22 alkyl, alkenyl, (C1-22 alkyl-substituted) aryl and the remainder is (OH-containing) C1-4 alkyl; R4 = **ester**, amido, (OH-containing) C2-6 alkylene; n = 1-3; Z-1 = anion], and nonionic surfactants, amphoteric surfactants, and/or anionic surfactants. Thus, 5% H2O2. 1% Me(CH2)10COO-1,4-C6H4SO3Na, 2% C12H25Me2N+C2H4N+Me3.2Cl-, 5% C12H25Me2N+CH2CH(OH)CH2.SO3-, 0.1% (HO)2P(O)C(OH)MeP(O)(OH)2, and balance H2O were mixed to give a composition exhibiting bleaching activity retention 97.3% after 5 mo at 50° and 80% relative humidity.

IT **175539-18-1P**
RL: IMF (Industrial manufacture); MOA (Modifier or additive use); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(additive; for liquid bleaching compns. containing hydrogen peroxide for textiles with good storage stability)

RN 175539-18-1 CAPLUS

CN 1,2-Ethanediaminium, N-[2-(dodecyldimethylammonio)ethyl]-N,N,N',N',N'-pentamethyl-, trichloride (9CI) (CA INDEX NAME)



● 3 Cl⁻

L17 ANSWER 9 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:704341 CAPLUS

DOCUMENT NUMBER: 121:304341

TITLE: Gas chromatographic separation of linear hydrocarbons on microporous organo-smectites

AUTHOR(S): Lao, Hongbai; Detellier, Christian

CORPORATE SOURCE: Ottawa-Carleton Chemistry Institute, University of Ottawa, Ottawa, ON, K1N 6N5, Can.

SOURCE: Clays and Clay Minerals (**1994**), 42(4), 477-81
CODEN: CLCMAB; ISSN: 0009-8604

PUBLISHER: Clay Minerals Society

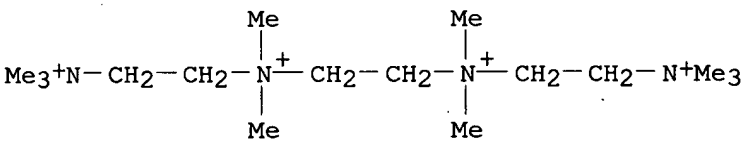
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of organo-montmorillonites and organo-hectorites were prepared by complete ion-exchange from the pure sodium form of the parent smectites. The organic cations were tetramethylammonium, tri-Me **quaternary** ammonium derivs. of lysine Me **ester** and ornithine Me **ester, quaternized** polyammonium cations, or tetraphenylphosphonium (TPP). These organo-smectites were used as packing material for gas chromatog. columns. Mixts. of light (C1-4) hydrocarbons could be separated The degree of separation depends on the presence of micropores or of organophilic mesopores. The BET surface area, the micropore and mesopore vols., as well as the size distribution of micropores and mesopores, were measured for several systems. As a general trend, the retention times of the light hydrocarbons decreased with increasing micropore volume In the case of TPP-montmorillonite, characterized by a large mesopore volume but for which no microporosity could be detected, separation of longer (C5-8) alkanes could also be achieved.

IT **108189-65-7D**, reaction products with hectorite and montmorillonite
RL: ARU (Analytical role, unclassified); PEP (Physical, engineering or chemical process); TEM (Technical or engineered material use); ANST (Analytical study); PROC (Process); USES (Uses)
(microporous organo-smectites as stationary phases for gas chromatog. separation of alkanes)

RN 108189-65-7 CAPLUS

CN 1,2-Ethanediaminium, N,N,N',N'-tetramethyl-N,N'-bis[2-(trimethylammonio)ethyl]- (9CI) (CA INDEX NAME)



L17 ANSWER 10 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:253366 CAPLUS
DOCUMENT NUMBER: 120:253366
TITLE: Compositions and methods for enhanced drug delivery
INVENTOR(S): Hale, Ron L.; Lu, Amy; Solas, Dennis; Selick, Harold E.; Oldenburg, Kevin R.; Zaffaroni, Alejandro C.
PATENT ASSIGNEE(S): Affymax Technologies N.V., Neth.
SOURCE: PCT Int. Appl., 155 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9325197	A1	19931223	WO 1993-US5631	19930611 <--
W: AT, AU, BB, BG, BR, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9345345	A1	19940104	AU 1993-45345	19930611 <--
EP 647133	A1	19950412	EP 1993-915319	19930611 <--
R: CH, DE, FR, GB, IT, LI, NL				

US 5607691	A	19970304	US 1995-449188		19950524 <--
PRIORITY APPLN. INFO.:			US 1992-898219	A2	19920612
			US 1993-9463	A2	19930127
			WO 1993-US5631	A	19930611
			US 1993-77296	B2	19930614
			US 1993-164293	B1	19931209

AB The present invention relates to methods of delivering pharmaceutical agents across membranes, including the skin layer or mucosal membranes of a patient. A pharmaceutical agent is covalently bonded to a chemical modifier, via a physiol. cleavable bond, such that the membrane transport and delivery of the agent is enhanced. Progesterone 3-{2-O-[10-O-(O-acetylcarnitinyl)decanoyl]glycolic acid} enol **ester** was prepared from progesterone by preparation of the enol acetate, reaction with 10-hydroxydecanoic acid, and reaction of the hydroxyl diester with 3-O-acetyl-L-carnitine acid chloride (preparation given). In vitro serum half-lives of some pharmaceutical agent-chemical modifier complexes are given.

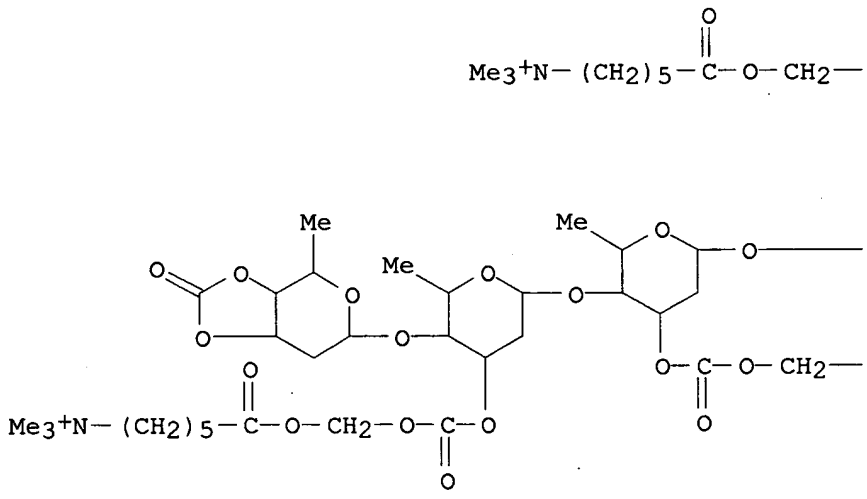
IT **154271-96-2**

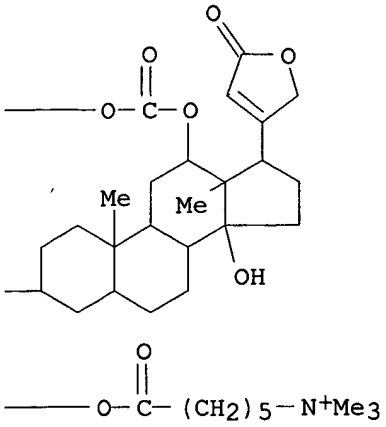
RL: BIOL (Biological study)
(as drug-chemical modifier conjugate through physiol. cleavable bond, in vitro serum half-life of)

RN 154271-96-2 CAPLUS

CN Card-20(22)-enolide, 3-[[O-3,4-O-carbonyl-2,6-dideoxy-β-D-ribo-hexopyranosyl-(1→4)-O-2,6-dideoxy-3-O-[[[[1-oxo-6-(trimethylammonio)hexyl]oxy]methoxy]carbonyl]-β-D-ribo-hexopyranosyl-(1→4)-2,6-dideoxy-3-O-[[[[1-oxo-6-(trimethylammonio)hexyl]oxy]methoxy]carbonyl]-β-D-ribo-hexopyranosyl]oxy]-14-hydroxy-12-[[[[[1-oxo-6-(trimethylammonio)hexyl]oxy]methoxy]carbonyl]oxy]-, tribromide, (3β,5β,12β)- (9CI) (CA INDEX NAME)

PAGE 1-A





●3 Br^-

=> d l17 11-20 ibib abs hitstr

L17 ANSWER 11 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1993:131746 CAPLUS
DOCUMENT NUMBER: 118:131746
TITLE: Shampoos containing cationic and anionic surfactants to impart improved hair conditioning properties
INVENTOR(S): Duffy, Michele; Bergmann, Wolfgang
PATENT ASSIGNEE(S): Curtis, Helene, Inc., USA
SOURCE: Eur. Pat. Appl., 42 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 511652	A1	19921104	EP 1992-107311	19920429 <--
EP 511652	B1	19951129		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
CA 2066885	AA	19921030	CA 1992-2066885	19920423 <--
CA 2066885	C	20020723		
IL 101682	A1	19961205	IL 1992-101682	19920423 <--
NO 9201640	A	19921030	NO 1992-1640	19920428 <--
NO 300355	B1	19970520		
AU 9215224	A1	19921105	AU 1992-15224	19920428 <--
AU 653216	B2	19940922		
ZA 9203084	A	19930127	ZA 1992-3084	19920428 <--
AT 130751	E	19951215	AT 1992-107311	19920429 <--
ES 2080369	T3	19960201	ES 1992-107311	19920429 <--
JP 06107525	A2	19940419	JP 1992-155568	19920430 <--

PRIORITY APPLN. INFO.: US 1991-692709 A 19910429
OTHER SOURCE(S): MARPAT 118:131746

AB A conditioning shampoo comprises (1) an anionic cleansing surfactant 1-15, (2) a polymeric cationic conditioning compound 0.1-2, (3) a cationic conditioning surfactant 0.2-10, (4) a fatty acid **ester** 0.1-3, and (5) water as carrier. A hair conditioner contained guar hydroxypropyltrimonium 1.50, ricinoleamidopropyl trimonium chloride (Surfactrol Q1) 1.65, linoleamidopropyl PG-dimonium chloride phosphate (Phospholipid EFA) 0.60, ammonium lauryl sulfate 6.14, ammonium lauryl ether sulfate 6.14, cetearyl octanoate (Purcellin oil) 2.00, and water

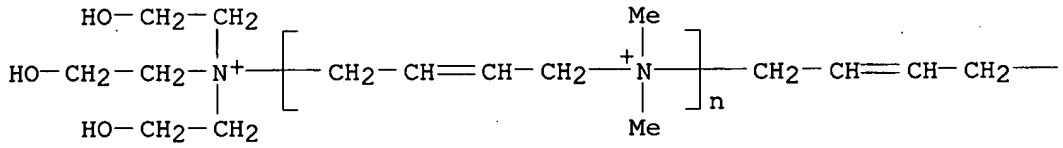
q.s. 100%.

IT **75345-27-6**, Polyquaternium 1
RL: BIOL (Biological study)
(hair conditioning shampoo containing anionic surfactants and fatty acid esters and)

RN 75345-27-6 CAPLUS

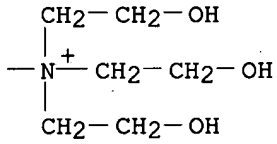
CN Poly[(dimethyliminio)-2-butene-1,4-diyl chloride], α-[4-[tris(2-hydroxyethyl)ammonio]-2-butenyl]-ω-[tris(2-hydroxyethyl)ammonio]-, dichloride (9CI) (CA INDEX NAME)

PAGE 1-A



●3 Cl^-

PAGE 1-B



L17 ANSWER 12 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:619747 CAPLUS
DOCUMENT NUMBER: 117:219747
TITLE: Cosmetic composition containing **quaternary** ammonium functionalized phosphate esters
INVENTOR(S): Ziegler, Philip D.; Cheney, Michael C.
PATENT ASSIGNEE(S): Chesebrough-Pond's USA Co., USA
SOURCE: U.S., 7 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5135748	A	19920804	US 1991-662680	19910228 <--
US 5169624	A	19921208	US 1991-662880	19910228 <--
CA 2061679	AA	19920829	CA 1992-2061679	19920221 <--
CA 2061679	C	19970603		
EP 501714	A2	19920902	EP 1992-301511	19920224 <--
EP 501714	A3	19930414		
EP 501714	B1	19970502		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, PT, SE				
AT 152347	E	19970515	AT 1992-301511	19920224 <--
ES 2102458	T3	19970801	ES 1992-301511	19920224 <--
BR 9200637	A	19921110	BR 1992-637	19920226 <--
AU 9211356	A1	19920903	AU 1992-11356	19920228 <--

AU 655229	B2	19941208			
JP 04338312	A2	19921125	JP 1992-43709		19920228 <--
JP 07014848	B4	19950222			
ZA 9201521	A	19930830	ZA 1992-1521		19920228 <--
KR 9701639	B1	19970213	KR 1992-3150		19920228 <--
PRIORITY APPLN. INFO.:			US 1991-662880		19910228
			US 1991-662680	A	19910228

OTHER SOURCE(S): MARPAT 117:219747

AB A cosmetic composition comprises title compds. [RCONH(CH2)3N+(Me)(Me)CH2CH(OH)CH2O]3PO 3X- (R = C5-17 alkyl, X = anion) 0.10-30, and a cationic polysaccharide 0.1-10%. These compns. are freeze-thaw cycle stable and exhibit unusual skin mildness properties. An emulsion contained cetyl alc. 2.5, glyceryl monostearate 1.5, iso-Pr palmitate 2, petrolatum 2, propylparaben 0.1, water 78.4, glycerin 10, Quatrisoft LM-200 (a cationic polysaccharide 0.25, Monaquat P-TS (phosphate tris alkylamido triquaternary compound) 3, antifoam AF 0.005, methylparaben 0.15, TiO2 0.1%.

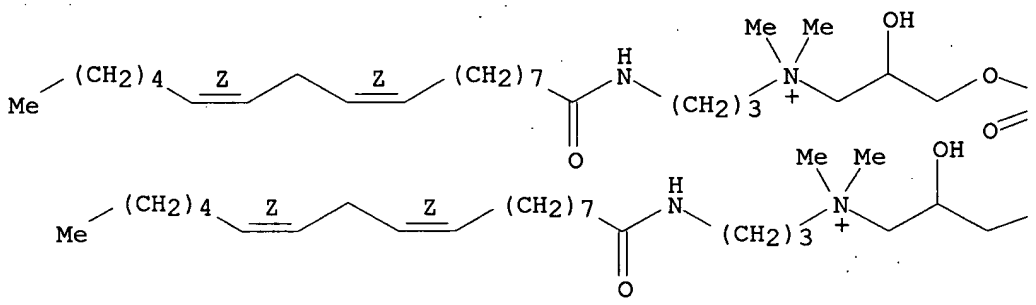
IT **144377-73-1**, Phospholipid EFA **144379-29-3**, Monaquat P-TS
RL: BIOL (Biological study)
(cosmetic composition containing cationic polysaccharides and)

RN 144377-73-1 CAPLUS

CN 4,6-Dioxa-14-aza-10-azonia-5-phosphadotriaconta-23,26-dien-1-aminium, 5-[3-[dimethyl[3-[[(9Z,12Z)-1-oxo-9,12-octadecadienyl]amino]propyl]ammonio]-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-15-oxo-N-[3-[[(9Z,12Z)-1-oxo-9,12-octadecadienyl]amino]propyl]-, trichloride, 5-oxide, (23Z,26Z)- (9CI) (CA INDEX NAME)

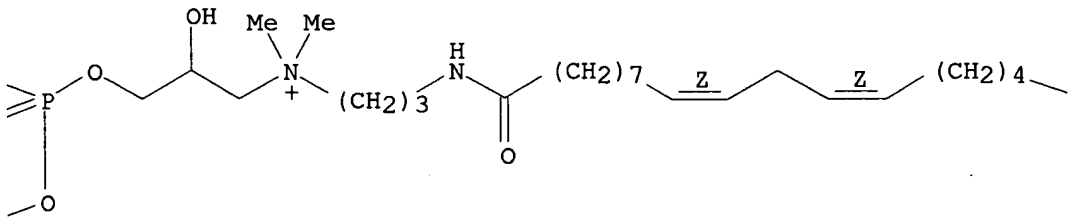
Double bond geometry as shown.

PAGE 1-A

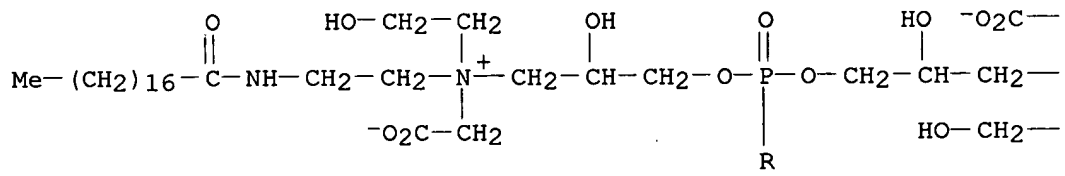


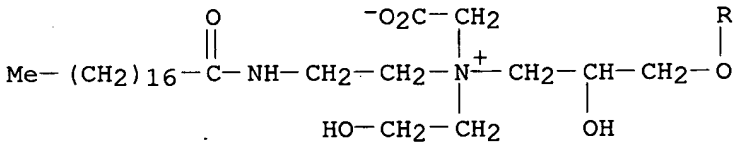
● 3 Cl^-

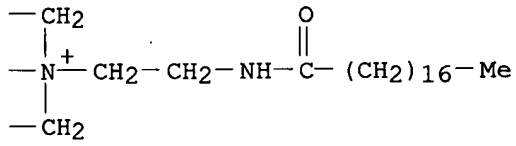
PAGE 1-B



RN 144379-29-3 CAPLUS
CN 4,6-Dioxa-13-aza-10-azonia-5-phosphahentriacontan-1-aminium, N,10-bis(carboxymethyl)-5-[3-[(carboxymethyl)(2-hydroxyethyl)[2-[(1-oxooctadecyl)amino]ethyl]ammonio]-2-hydroxypropoxy]-2,8-dihydroxy-N,10-bis(2-hydroxyethyl)-14-oxo-N-[2-[(1-oxooctadecyl)amino]ethyl]-, tris(inner salt), 5-oxide (9CI) (CA INDEX NAME)





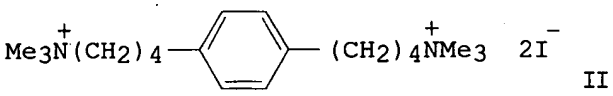


L17 ANSWER 13 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1991:514182 CAPLUS
DOCUMENT NUMBER: 115:114182
TITLE: Preparation of **quaternary** ammonium compounds as muscle relaxants
INVENTOR(S): Kimura, Masayasu; Naito, Kenji; Sakuma, Osamu; Morita, Tadashi
PATENT ASSIGNEE(S): Tobishi Pharmaceutical Co., Ltd., Japan
SOURCE: Ger. Offen., 38 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4010925	A1	19901011	DE 1990-4010925	19900404 <--

JP 02268142	A2	19901101	JP 1989-87889	19890410 <--
CA 2013432	AA	19901010	CA 1990-2013432	19900329 <--
CH 679581	A	19920313	CH 1990-1173	19900405 <--
FR 2645532	A1	19901012	FR 1990-4431	19900406 <--
US 5093370	A	19920303	US 1990-506862	19900409 <--
GB 2230263	A1	19901017	GB 1990-8074	19900410 <--

PRIORITY APPLN. INFO.: JP 1989-87889 A 19890410
OTHER SOURCE(S): MARPAT 115:114182
GI



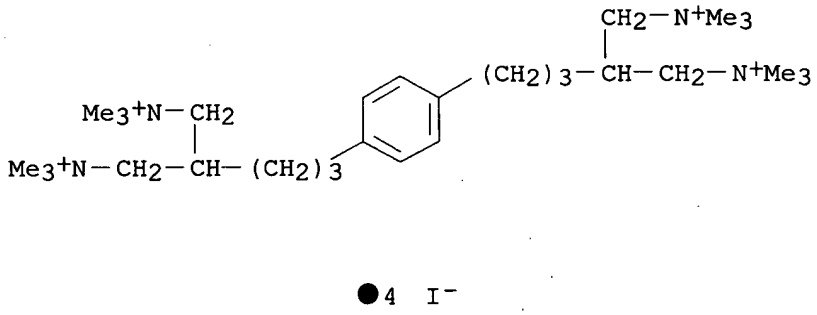
II

AB [R2R3QZ(CH2)a[CH(CH2A)CH2]bA]m+] (R4)m- [I; Z = CH2, alkylene(oxy), alkynylene, CO, CO2, alkylene(carbonyloxy), CHOR5, alkylenecarbonyl, O, S, SO, SO2, hydroxyalkyl; R2 = H, hydroxyalkyl, formyl, alkylcarbonyl, NO2, NHR6; R3 = H, Z(CH2)a[CH(CH2A)CH2]b; R4 = anion; R5, R6 = H, Ac; A = **quaternary** ammonium group; Q = trivalent benzene, naphthalene, or biphenyl ring, trivalent ethane radical; a = 1-8; b = 0, 1; m = 1-4] were prepared by reaction of halo derivs. R2R3QZ(CH2)a[CH(CH2A)CH2]bR7 (R7 = halo, reactive **ester** group, other symbols as defined above) with tertiary amines. Thus, bromination of 11.5 g 1,4-bis(4-hydroxybutyl)benzene (preparation from p-diiodobenzene given) by PBr3 gave 13.1 g 1,4-bis(4-bromobutyl)benzene which (3.48 g) was stirred 3.5 h at room temperature with 9 mL 50% Me2NH to give 2.70 g 1,4-bis(dimethylamino) analog. This (3.1 g) was refluxed 2.5 in MeOH with 7.2 g MeI to give 3.57 g title compound II. The latter in vitro inhibited muscle contractions induced by elec. shock with IC50 of 22.8 μM vs. 25.2 and 101 μM for succinylcholine and decamethonium, resp. Approx. 42 I were prepared

IT **134519-58-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as muscle relaxant)

RN 134519-58-7 CAPLUS

CN 1,4-Benzenedipentanaminium, N,N,N,N',N',N'-hexamethyl-β,β'-bis[(trimethylammonio)methyl]-, tetraiodide (9CI) (CA INDEX NAME)



L17 ANSWER 14 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:	1991:209601 CAPLUS
DOCUMENT NUMBER:	114:209601
TITLE:	Bleaching detergent compositions containing sulfonate salts
INVENTOR(S):	Aoyanagi, Muneo; Kuroda, Mutsumi; Araki, Hiroyuki; Taguchi, Akio

PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

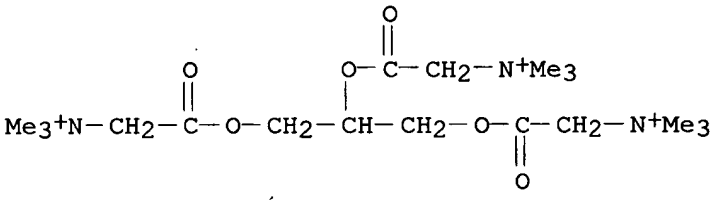
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02229895	A2	19900912	JP 1989-230773	19890906 <--
PRIORITY APPLN. INFO.:			JP 1988-237369 A1	19880921

OTHER SOURCE(S): MARPAT 114:209601

AB Title compns. comprise 3-30% peroxides generating H2O2 in aqueous solns., 0.1-30% activators which react with H2O2 to generate cationic group-containing organic peroxy acids, and 10-50% mixts. (9/1-1/3) of alkylbenzenesulfonate salts and α-sulfo fatty acid **ester** salts. Thus, a composition containing Na dodecylbenzenesulfonate 22, hydrogenated palm oil fatty acid Me **ester** Na sulfonate 3, Na silicate 5, Na2CO3 10, 4A zeolite 25, Na2S2O6 10, NCCH2N+Me2CH2CH2N+Me2CH2CN 2Cl- 5, PEG 2, protease 2, and H2O 5%, with the remainder being Na2SO4 was used to wash and bleach a tea-stained cotton cloth.

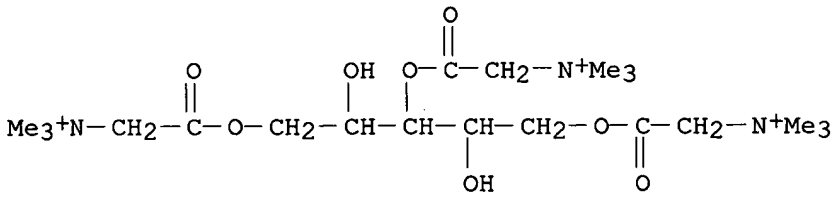
IT **130631-35-5 132787-32-7**
RL: CAT (Catalyst use); USES (Uses)
(activators, for peroxide bleaching agents, in laundry detergents)

RN 130631-35-5 CAPLUS
CN Ethanaminium, 2,2',2''-[1,2,3-propanetriyltris(oxy)]tris[N,N,N-trimethyl-2-oxo-, trichloride (9CI) (CA INDEX NAME)



● 3 Cl^-

RN 132787-32-7 CAPLUS
CN Pentitol, 1,3,5-tris[(trimethylammonio)acetate], trichloride (9CI) (CA INDEX NAME)



● 3 Cl^-

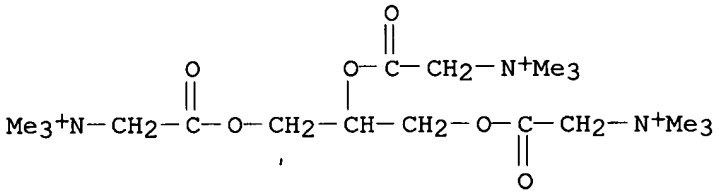
L17 ANSWER 15 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1990:614309 CAPLUS
DOCUMENT NUMBER: 113:214309
TITLE: Bleaching composition
INVENTOR(S): Sotoya, Kohshiro; Ogura, Nobuyuki; Aoyagi, Muneo; Murata, Moriyasu
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Eur. Pat. Appl., 18 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 371809	A1	19900606	EP 1989-312492	19891130 <--
EP 371809	B1	19940928		
R: DE, ES, FR, GB				
JP 02147698	A2	19900606	JP 1988-303161	19881130 <--
JP 06096719	B4	19941130		
US 5093022	A	19920303	US 1989-441941	19891127 <--
ES 2059786	T3	19941116	ES 1989-312492	19891130 <--
PRIORITY APPLN. INFO.:			JP 1988-303161 A	19881130
OTHER SOURCE(S):		MARPAT 113:214309		

AB Compds. R1N+R2R3R4COL X- (R1-3 = alkyl, alkenyl, alkaryl; R4 = alkylene, phenylene, etc.; L = OC6H4CO2R5, OC6H4NR6R7, O-p-C6H4CR6R7-p-C6H4OY, ON:CR5R6, succinimidooxy, etc.; R5 = alkyl; R6-7 = H, alkyl; Y = H, COR4N+R1R2R3; X- = anion) are useful as activators for peroxygen bleaching agents, especially in laundry detergents. The activator Me3N+(CH2)3CO2-p-C6H4CO2Me Cl- was more effective than (Ac2NCH2)2 in the bleaching of tea-stained fabrics with Na percarbonate.

IT **130631-35-5**
RL: USES (Uses)
(bleaching activators, for peroxygen compds. in laundrying)

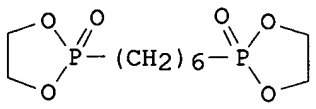
RN 130631-35-5 CAPLUS
CN Ethanaminium, 2,2',2''-[1,2,3-propanetriyltris(oxy)]tris[N,N,N-trimethyl-2-oxo-, trichloride (9CI) (CA INDEX NAME)



●3 Cl⁻

L17 ANSWER 16 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1990:552621 CAPLUS
DOCUMENT NUMBER: 113:152621
TITLE: Choline esters of alkylenebisphosphonic acids
AUTHOR(S): Bikchurina, L. Kh.; Yumagulova, R. Kh.; Khalilov, L. M.; Vasil'eva, E. V.; Leplyanin, G. V.
CORPORATE SOURCE: Inst. Khim., Ufa, USSR
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (

1990), (6), 1424-9
CODEN: IASKA6; ISSN: 0002-3353
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 113:152621
GI



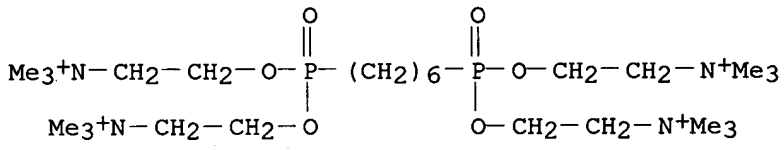
I

AB Reaction of (CH2)6[P(O)Cl2]2 with HOCH2CH2OH and HOCH2CH2Cl gave esters I and (CH2)6[P(O)(OCH2CH2Cl)2]2 resp. which on **quaternization** with NMe3 gave (CH2)6[P(O)(O-)OCH2CH2N+Me3]2 and (CH2)6[P(O)(OCH2N+Me3 Cl-)2]2 resp.

IT **129623-00-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 129623-00-3 CAPLUS

CN 3,12-Dioxa-4,11-diphosphatetradecane-1,14-diaminium, N,N,N,N',N',N'-hexamethyl-4,11-bis[2-(trimethylammonio)ethoxy]-, tetrachloride, 4,11-dioxide (9CI) (CA INDEX NAME)



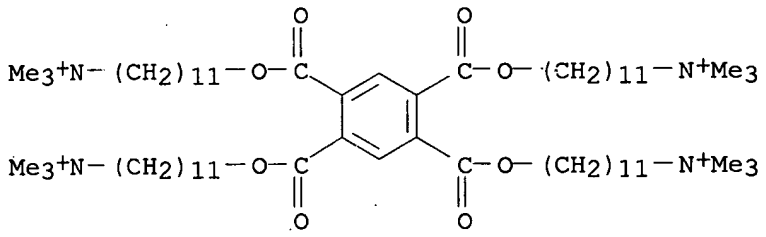
● 4 Cl^-

L17 ANSWER 17 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:119376 CAPLUS
DOCUMENT NUMBER: 108:119376
TITLE: Structural variations in amphiphiles: discoidal multivalent cations
AUTHOR(S): Keller-Griffith, R.; Ringsdorf, H.; Vierengel, A.
CORPORATE SOURCE: Inst. Org. Chem., Univ. Mainz, Mainz, D-6500, Fed. Rep. Ger.
SOURCE: Colloid and Polymer Science (**1986**), 264(11), 924-35
CODEN: CPMSB6; ISSN: 0303-402X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Fourteen cationic multipolar amphiphiles were synthesized with pyridinium or trimethylammonium head groups. The hydrophobic cores are planar ring systems (benzene or triphenylene) to which 2, 3, 4, or 6 decylene or undecylene alkyl chains are attached by **ester** linkages. The hydrophilic head groups are bound to the outer ends of the alkyl chains. The aggregation of the mols. in water into micelles and lyotropic liquid crystals was studied. Hexagonal phases are preferred to lamellar phases by these amphiphiles and in more dilute solns. some of these multipolar amphiphiles form cylindrical micelles.

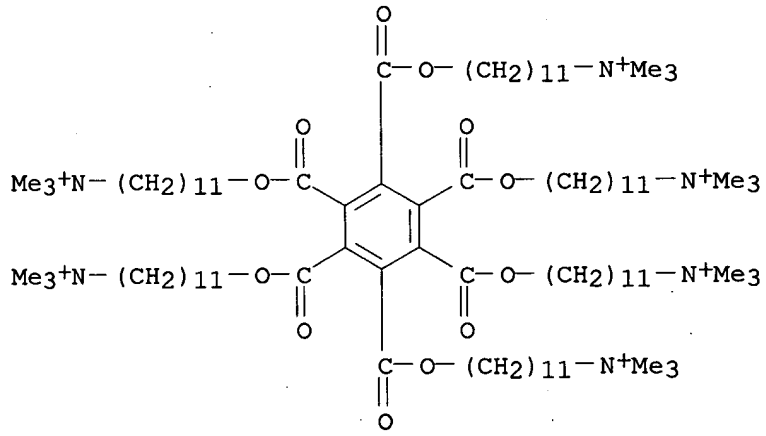
IT **106349-87-5 106349-88-6 113339-63-2**
113339-65-4 113339-66-5 113339-67-6
113339-70-1
RL: PRP (Properties)
(micelle and liquid crystal aggregation properties of aqueous)

RN 106349-87-5 CAPLUS
CN 1-Undecanaminium, 11,11',11'',11'''-[1,2,4,5-benzenetetrayltetrakis(carbonyloxy)]tetrakis[N,N,N-trimethyl-, tetrabromide (9CI) (CA INDEX NAME)



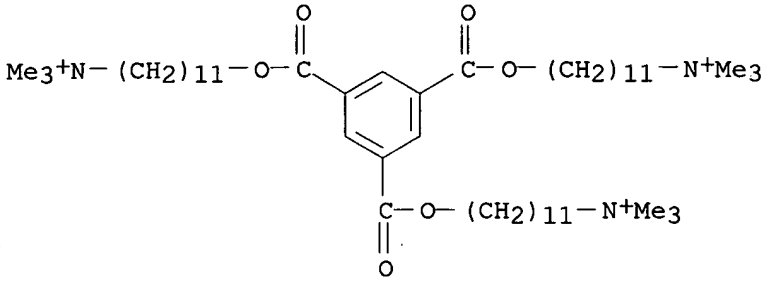
●4 Br^-

RN 106349-88-6 CAPLUS
CN 1-Undecanaminium, 11,11',11'',11''',11'''',11'''''-[1,2,3,4,5,6-benzenehexaylhexakis(carbonyloxy)]hexakis[N,N,N-trimethyl-, hexabromide (9CI) (CA INDEX NAME)



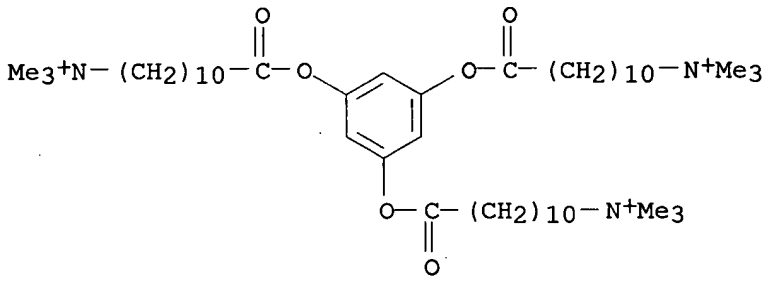
●6 Br^-

RN 113339-63-2 CAPLUS
CN 1-Undecanaminium, 11,11',11''-[1,3,5-benzenetriyltris(carbonyloxy)]tris[N,N,N-trimethyl-, tribromide (9CI) (CA INDEX NAME)



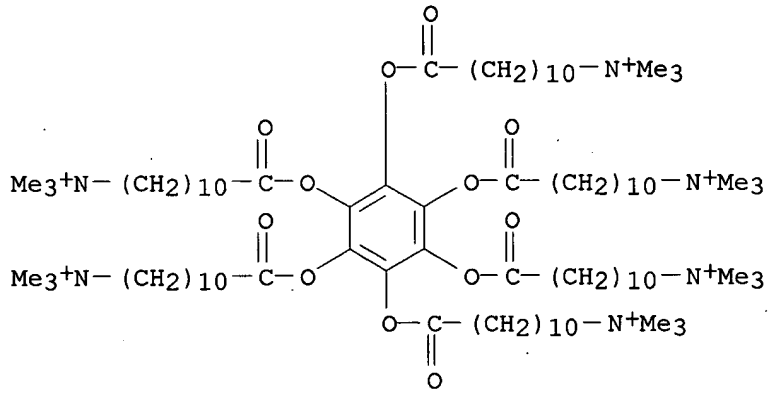
●3 Br^-

RN 113339-65-4 CAPLUS
CN 1-Undecanaminium, 11,11',11''-[1,3,5-benzenetriyltris(oxy)]tris[N,N,N-trimethyl-11-oxo-, tribromide (9CI) (CA INDEX NAME)



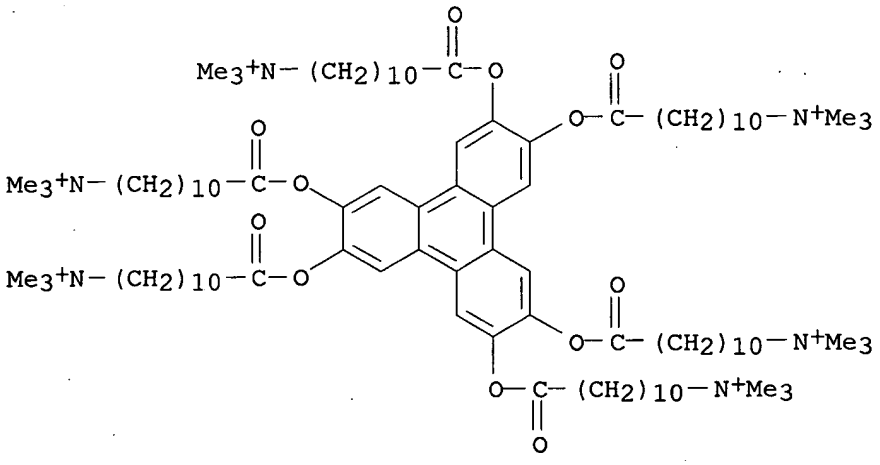
●3 Br

RN 113339-66-5 CAPLUS
CN 1-Undecanaminium, 11,11',11'',11''',11'''',11''''',11'''''-[1,2,3,4,5,6-benzenehexaylhexakis(oxy)]hexakis[N,N,N-trimethyl-11-oxo-, hexabromide (9CI) (CA INDEX NAME)



●6 Br^-

RN 113339-67-6 CAPLUS
CN 1-Undecanaminium, 11,11',11'',11''',11'''',11'''''-[2,3,6,7,10,11-triphenylenehexaylhexakis(oxy)]hexakis[N,N,N-trimethyl-11-oxo-, hexabromide (9CI) (CA INDEX NAME)

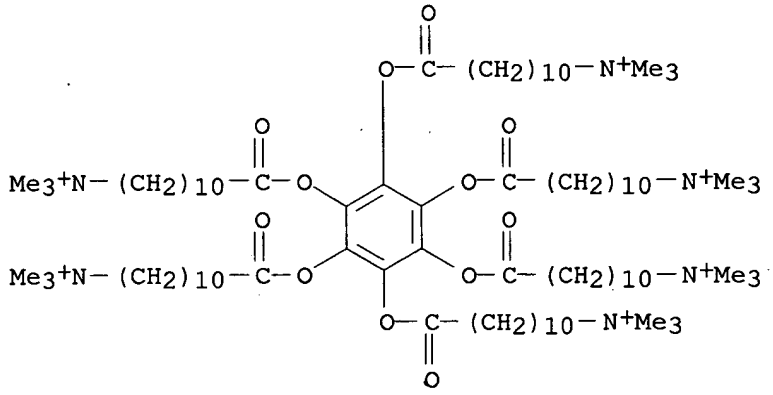


●6 Br^-

RN 113339-70-1 CAPLUS
CN 1-Undecanaminium, 11,11',11'',11''',11'''',11'''''-[1,2,3,4,5,6-benzenehexaylhexakis(oxy)]hexakis[N,N,N-trimethyl-11-oxo-, salt with 2-hydroxybenzoic acid (1:6) (9CI) (CA INDEX NAME)

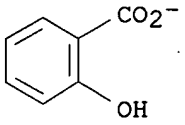
CM 1

CRN 113339-69-8
CMF C90 H174 N6 O12



CM 2

CRN 63-36-5
CMF C7 H5 O3

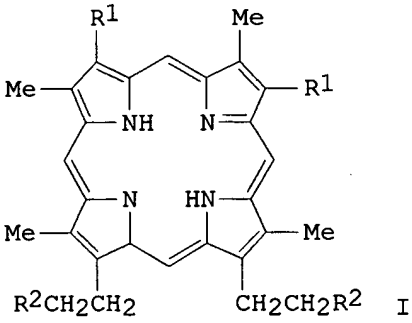


L17 ANSWER 18 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:75115 CAPLUS
DOCUMENT NUMBER: 108:75115
TITLE: Preparation and formulation of porphyrin derivatives useful for the diagnosis and treatment of cancer
INVENTOR(S): Fukuda, Yozo; Otani, Takuzo; Yamada, Haruo; Sawada, Michikazu; Aizawa, Katsuo; Uchimoto, Mari; Karasawa, Michito
PATENT ASSIGNEE(S): Hamari Chemicals, Ltd., Japan
SOURCE: Eur. Pat. Appl., 33 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 233701	A2	19870826	EP 1987-300374	19870116 <--
EP 233701	A3	19880921		
EP 233701	B1	19910814		
R: CH, DE, FR, GB, IT, LI				
JP 62167783	A2	19870724	JP 1986-8789	19860117 <--
JP 07020963	B4	19950308		
JP 62205082	A2	19870909	JP 1986-46000	19860303 <--
JP 07014942	B4	19950222		
JP 63145283	A2	19880617	JP 1986-291904	19861208 <--

PRIORITY APPLN. INFO.:
JP 1986-8789 A 19860117
JP 1986-46000 A 19860303
JP 1986-291904 A 19861208

GI



I

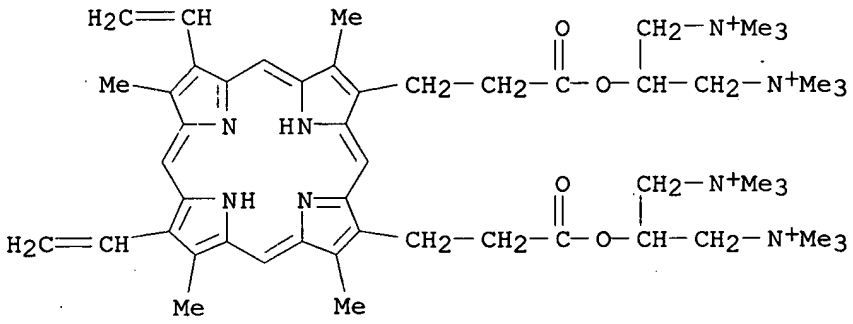
AB Title compds. I [R1 = H, C1-4 alkyl, ethenyl, C2-4Q, Q = di(C1-4-alkyl)amino, tri(C1-4-alkyl)ammonium halide, pyridinio-, quinolinioalkyl halide; R2 = HO2C, C1-4 alkoxycarbonyl, COZ(CmH2m)Q, COZCH(CmH2mQ)2, CH2Q (Z = O, S, HN; m = 1-23]. 7,12-Diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropionic acid in CH2Cl2 was treated with (COCl)2 to give the acid chloride which was esterified with Me2NCH2CH2OH to the **ester**, which in CH2Cl2 was **quaternized** with MeI to give I [R1 = ethenyl; R2 =

[2-(trimethylammonio)ethoxy]carbonyl diiodide] (II). MKSA cells from mouse nephradenoma transplanted on a mouse's back, were treated with II at 20 mg/kg, i.v., and excimer laser irradiated, whereby the tumor disappeared after 3 days.

IT **112635-97-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as anticancer drug)

RN 112635-97-9 CAPLUS

CN 1,3-Propanediaminium, 2,2'-[(7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-diyl)bis[(1-oxo-3,1-propanediyl)oxy]]bis[N,N,N,N',N',N'-hexamethyl-, tetraiodide (9CI) (CA INDEX NAME)



●4 I^-

L17 ANSWER 19 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1987:556318 CAPLUS
DOCUMENT NUMBER: 107:156318
TITLE: Auxiliary agent combination and its use as a textile-finishing agent
INVENTOR(S): Abel, Heinz; Topfl, Rosemarie; Gunter, Franz
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Eur. Pat. Appl., 24 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 225281	A1	19870610	EP 1986-810500	19861103 <--
EP 225281	B1	19890614		
R: BE, CH, DE, FR, GB, IT, LI				
US 4728337	A	19880301	US 1986-925027	19861030 <--
CA 1278402	A1	19910102	CA 1986-522298	19861106 <--
AU 8664951	A1	19870514	AU 1986-64951	19861107 <--
AU 589463	B2	19891012		
ZA 8608485	A	19870624	ZA 1986-8485	19861107 <--
JP 62117887	A2	19870529	JP 1986-264918	19861108 <--
JP 01027189	B4	19890526		

PRIORITY APPLN. INFO.: CH 1985-4802 A 19851108

AB The **quaternary** salts [R1COX1Z1N(R3)(R4)QN(R5)(R6)Z2X2COR2]2+ 2Y- (Q = alkylene, optionally containing O or bearing OH; R1, R2 = C6-24 aliphatic group; R3-6 = alkyl, hydroxyalkyl, alkoxyalkyl; X1, X2 = O, HH; Z1, Z2 = alkylene; Y = anion of a strong acid] are useful in finishing textiles,

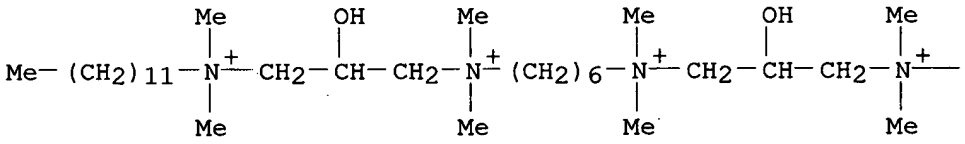
especially post-treatment in wool dyeing. Chlorinated wool was dyed with a mixture of chrome, cobalt, and azo dyes, rinsed, heated in an aqueous solution of
0.6% HOCH[CH2N(Me)2(CH2)3NHCOC21H43+]2.2Cl- (I) and 0.6% 4,4'-bis(chloromethyl)biphenyl-N,N,N',N'-tetramethyl-1,6-hexanediamine copolymer (II) at bath ratio 1:30, pH 5, and 40° for 10 min to give a dyeing with fastness to potting, washing, and light 4, 5, and 4-5, resp., and no dry or wet soiling; vs. 4, 5, 4-5, and strong, resp., without I, and 1, 3-4, 4-5, and none, resp., without I and II.

IT **110675-15-5**
RL: USES (Uses)
(afterfinishes, for dyed wool)

RN 110675-15-5 CAPLUS

CN 1,6-Hexanediaminium, N,N'-bis[3-(dodecyldimethylammonio)-2-hydroxypropyl]-N,N,N',N'-tetramethyl-, tetrachloride (9CI) (CA INDEX NAME)

PAGE 1-A



●4 Cl⁻

PAGE 1-B

—(CH2)11—Me

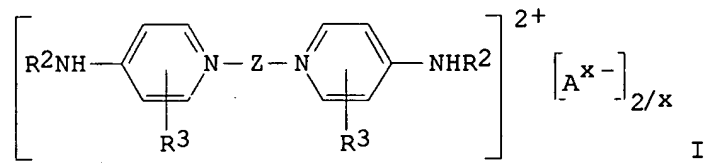
L17 ANSWER 20 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1986:230452 CAPLUS
DOCUMENT NUMBER: 104:230452
TITLE: Antimicrobial compositions for disinfecting surfaces
INVENTOR(S): Gorman, William George; Popp, Karl Frederick
PATENT ASSIGNEE(S): Sterling Drug Inc., USA
SOURCE: Eur. Pat. Appl., 24 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 161425	A2	19851121	EP 1985-103318	19850321 <--
EP 161425	A3	19860226		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
AU 8539855	A1	19850926	AU 1985-39855	19850314 <--
JP 60226802	A2	19851112	JP 1985-52175	19850315 <--
ZA 8502023	A	19851127	ZA 1985-2023	19850319 <--
FI 8501139	A	19850924	FI 1985-1139	19850321 <--
NO 8501149	A	19850924	NO 1985-1149	19850321 <--

DK 8501321	A	19850924	DK 1985-1321		19850322 <--
IL 74695	A1	19880630	IL 1985-74695		19850322 <--
PRIORITY APPLN. INFO.:			US 1984-592664	A	19840323

GI



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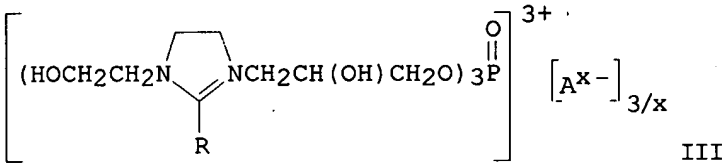


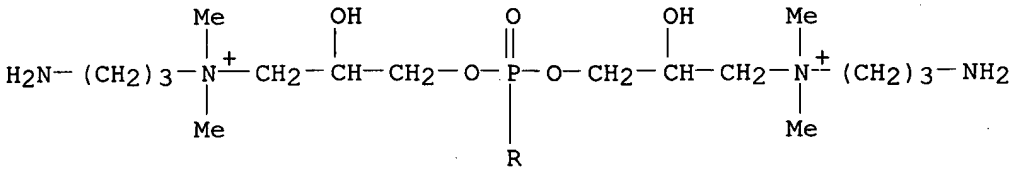
III

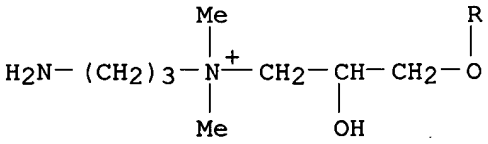
AB The title compns. contain a bisbiguanide, RR1NC(:NH)NHC(:NH)NH(CH2)nNHC(:NH)NHC(:NH)NRR1 [R = C6-16 alkyl, cycloalkyl, polycyclic alkyl, alkylcycloalkyl, cycloalkylalkyl, 4-(2,2-dichlorocyclopropyl)phenyl, (un)substituted Ph; R1 = H; RR1 = 3-azabicyclo[3.2.2]nonyl; n = 3-9], or a bis[4-(substituted-amino)-1-pyridinium]alkane I (R2 = C6-18 alkyl, C5-7 cycloalkyl, (un)substituted PhCH2, Ph; R3 = H, alkyl; Z = C4-18 alkylene; A = anion; x = valence of anion] especially octenidine-HCl, and 1 or more **quaternary** ammonium phosphate **ester** surfactants [(R4CONHCH2CH2CH2NMe2CH2CH(OH)CH2O)3PO]3+ [Ax-]3/x (II) and III (R4 = C5-17 alkyl; A, x as before) and an aqueous vehicle and addnl. 1 or more polyethylene glycol **ester** surfactant and a **quaternary** nitrogen-containing cellulose ether. Thus, an antimicrobial skin cleansing composition was formulated containing octenidine-HCl 2.0, cocamidopropyl PG-dimonium chloride phosphate (II, R4CO = coco acyl) 6.0, PEG-glyceryl cocoate 11.0, NaH2PO4 0.276, di-Na EDTA 0.1, perfume 0.1, dye 0.005, NaOH to make pH 7.2, and H2O to 100% by weight Porcine skin disks inoculated with Staphylococcus epidermis were immersed in the above composition and the number of surviving bacteria was determined The results showed a significant mean log10 count redns. of bacteria on the disks.

IT **75464-22-1D**, N-coco acyl derivs.
RL: BIOL (Biological study)
(skin disinfectant compns. containing surfactants and)

RN 75464-22-1 CAPLUS

CN 4,6-Dioxa-10-azonia-5-phosphatridecan-1-aminium, 13-amino-N-(3-aminopropyl)-5-[3-[(3-aminopropyl)dimethylammonio]-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-, trichloride, 5-oxide (9CI) (CA INDEX NAME)





●3 Cl⁻

=> d l17 21-30 ibib abs hitstr

L17 ANSWER 21 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1982:533355 CAPLUS
DOCUMENT NUMBER: 97:133355
TITLE: Oily, foaming agent with a liquid phase for care of keratin materials and the skin
INVENTOR(S): Grollier, Jean Francois; Allec, Josiane
PATENT ASSIGNEE(S): Oreal S. A. , Fr.
SOURCE: Ger. Offen., 47 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3150338	A1	19820715	DE 1981-3150338	19811218 <--
DE 3150338	C2	19890511		
BE 891528	A1	19820618	BE 1981-206873	19811218 <--
FR 2496458	A1	19820625	FR 1981-23773	19811218 <--
FR 2496458	B1	19870717		
GB 2091100	A	19820728	GB 1981-38210	19811218 <--
GB 2091100	B2	19850227		
JP 57128618	A2	19820810	JP 1981-205048	19811218 <--
JP 02049284	B4	19901029		
CA 1175357	A1	19841002	CA 1981-392613	19811218 <--
US 4488564	A	19841218	US 1981-331904	19811218 <--
CH 651468	A	19850930	CH 1981-8120	19811218 <--
PRIORITY APPLN. INFO.:			LU 1980-83020 A	19801219

AB An oil-containing foaming cleanser for skin and hair contains an oil liquid at ambient temperature 5-85, a surfactant soluble in the oil 15-95, a cationic compound 0.5-10, and H2O 0.1-5%. The oil may be plant, animal, or mineral, or synthetic glyceride or fatty acid **ester**, or fatty alc. The oil-soluble surfactant is anionic, with the acid group neutralized with an amine, or nonionic, and (or) alkanolamide. The cationic compound is a polymer containing polyamino, polyaminoamide, or **quaternary** ammonium groups as part of the polymer chain. Thus, a shampoo contained: Texapon

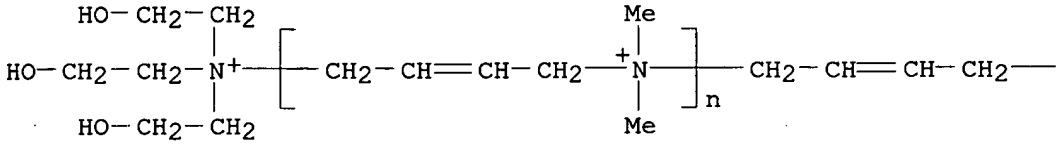
WW 99 [83045-95-8] 15, paraffin oil 25, Polymer P1 [68393-49-7] (60% aqueous solution) 3, perfume, antioxidants, and olive oil to 100 g. In use, 20 mL was applied to wet hair, worked in, allowed to stand 10 min, and rinsed to give soft hair that is easily detangled.

IT **75345-27-6**
RL: BIOL (Biological study)
(shampoos containing oils and)

RN 75345-27-6 CAPLUS

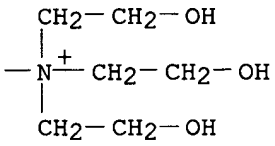
CN Poly[(dimethyliminio)-2-butene-1,4-diyl chloride], α-[4-[tris(2-hydroxyethyl)ammonio]-2-butenyl]-ω-[tris(2-hydroxyethyl)ammonio]-, dichloride (9CI) (CA INDEX NAME)

PAGE 1-A



●3 Cl^-

PAGE 1-B



L17 ANSWER 22 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1981:426943 CAPLUS
DOCUMENT NUMBER: 95:26943
TITLE: Surfactants useful in conditioning and cleaning agents
INVENTOR(S): Lindeman, Martin K. O.; Stutzman, Ralph; Verdicchio, Robert J.
PATENT ASSIGNEE(S): Johnson and Johnson Baby Products Co., USA
SOURCE: Ger. Offen., 30 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3027944	A1	19810219	DE 1980-3027944	19800723 <--
AU 8059761	A1	19810129	AU 1980-59761	19800630 <--
AU 535124	B2	19840301		
FR 2461517	A1	19810206	FR 1980-15681	19800716 <--
CA 1165659	A1	19840417	CA 1980-356656	19800721 <--
GB 2055119	A	19810225	GB 1980-23868	19800722 <--
GB 2055119	B2	19830420		
JP 56020095	A2	19810225	JP 1980-99448	19800722 <--
JP 02025958	B4	19900606		
BR 8004565	A	19810310	BR 1980-4565	19800722 <--

ES 493596	A1	19810616	ES 1980-493596		19800722 <--
ZA 8004422	A	19820224	ZA 1980-4422		19800722 <--
AT 8003794	A	19840215	AT 1980-3794		19800722 <--
AT 375957	B	19840925			

PRIORITY APPLN. INFO.: US 1979-59837 A 19790723

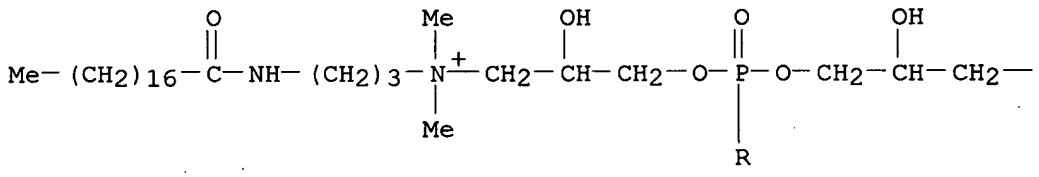
AB **Quaternary** ammonioalkyl phosphates are conditioning agents and detergents in shampoos, wool cleansers, etc., which are nonirritating to skin and eyes. Thus, a shampoo contains OP[OCH2CH(OH)CH2N+Me2C18H37 Cl-]3 [**77195-38-1**] 2, OP[OCH2CH(OH)CH2N+Me2C12H25 Cl-]3 [**77195-39-2**] 0.1, C12H25OSO3Na 12, C11H23CON(CH2CH2OH)2 4, and perfume-dye-water 81.9%.

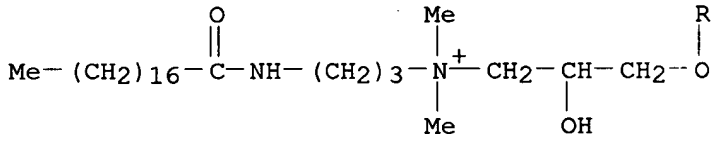
IT **75464-24-3 77195-35-8 77195-36-9 77195-37-0 77195-38-1 77195-39-2**
RL: TEM (Technical or engineered material use); USES (Uses) (surfactants, nonirritating)

RN 75464-24-3 CAPLUS

CN 4,6-Dioxa-14-aza-10-azonia-5-phosphadotriacontan-1-aminium, 5-[3-[dimethyl[3-[(1-oxooctadecyl)amino]propyl]ammonio]-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-15-oxo-N-[3-[(1-oxooctadecyl)amino]propyl]-, trichloride, 5-oxide (9CI) (CA INDEX NAME)

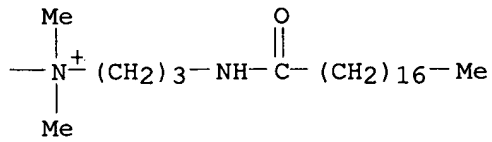
PAGE 1-A





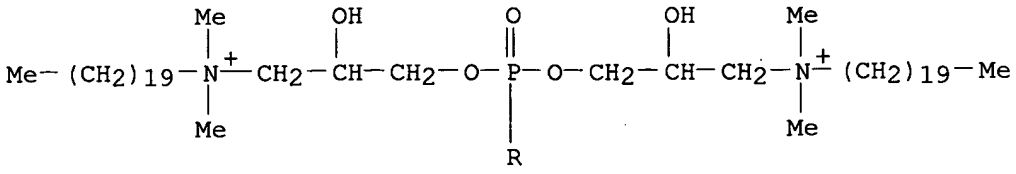
●3 Cl⁻

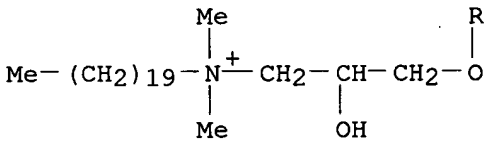
PAGE 1-B



RN 77195-35-8 CAPLUS

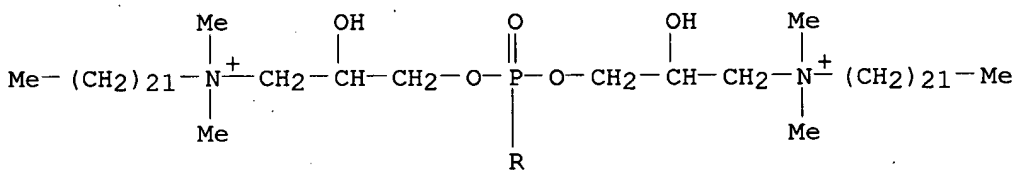
CN 4,6-Dioxa-10-azonia-5-phosphatriacontan-1-aminium, N-eicosyl-5-[3-(eicosyldimethylammonio)-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-, trichloride, 5-oxide (9CI) (CA INDEX NAME)

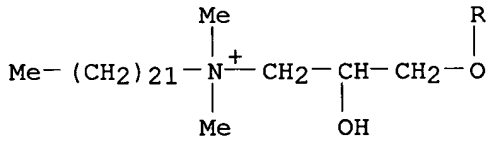




●3 Cl^-

RN 77195-36-9 CAPLUS
CN 4,6-Dioxa-10-azonia-5-phosphadotriacontan-1-aminium, N-docosyl-5-[3-(docosyldimethylammonio)-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-, trichloride, 5-oxide (9CI) (CA INDEX NAME)

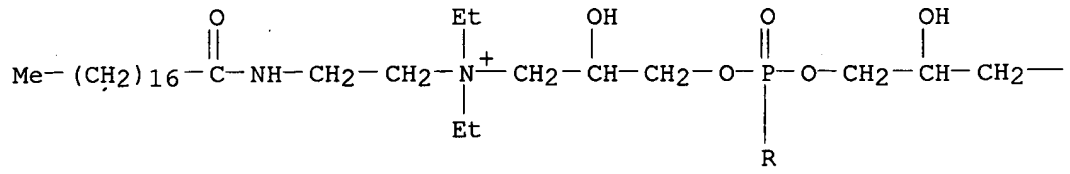


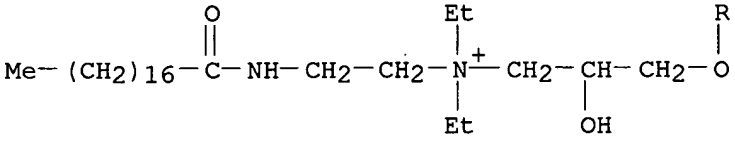


●3 Cl^-

RN 77195-37-0 CAPLUS
CN 4,6-Dioxa-13-aza-10-azonia-5-phosphahentriacontan-1-aminium, 5-[3-[diethyl[2-[(1-oxooctadecyl)amino]ethyl]ammonio]-2-hydroxypropoxy]-N,N,10,10-tetraethyl-2,8-dihydroxy-14-oxo-N-[2-[(1-oxooctadecyl)amino]ethyl]-, trichloride, 5-oxide (9CI) (CA INDEX NAME)

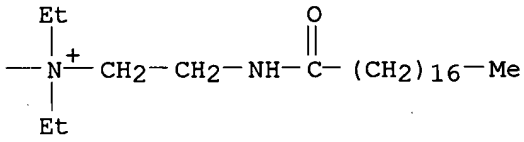
PAGE 1-A



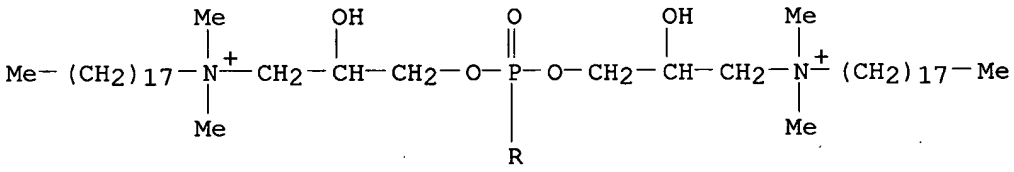


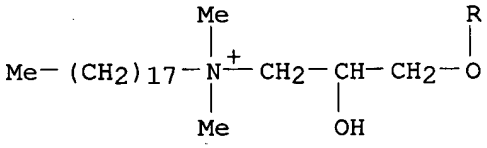
● 3 Cl^-

PAGE 1-B



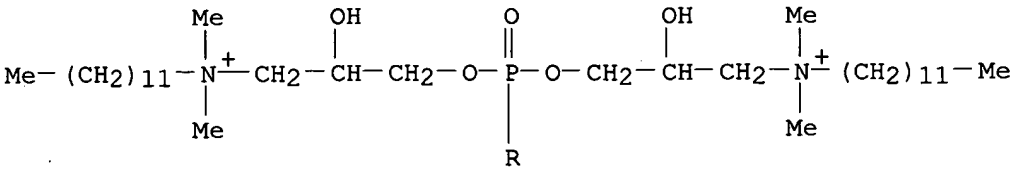
RN 77195-38-1 CAPLUS
CN 4,6-Dioxa-10-azonia-5-phosphaoctacosan-1-aminium, 5-[3-(dimethyloctadecylammonio)-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-N-octadecyl-, trichloride, 5-oxide (9CI) (CA INDEX NAME)

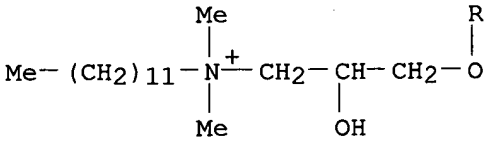




● 3 Cl^-

RN 77195-39-2 CAPLUS
CN 4,6-Dioxa-10-azonia-5-phosphadocosan-1-aminium, N-dodecyl-5-[3-(dodecyldimethylammonio)-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-, trichloride, 5-oxide (9CI) (CA INDEX NAME)





●3 Cl^-

L17 ANSWER 23 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1981:191667 CAPLUS
DOCUMENT NUMBER: 94:191667
TITLE: Cationic phosphoric acid triesters and their use
INVENTOR(S): Lindemann, Martin K. O.; Lukenbach, Elvin R.; Verdicchio, Robert J.
PATENT ASSIGNEE(S): Johnson and Johnson Baby Products Co., USA
SOURCE: Ger. Offen., 23 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3027943	A1	19810219	DE 1980-3027943	19800723 <--
DE 3027943	C2	19880901		
AU 8059762	A1	19810129	AU 1980-59762	19800630 <--
AU 536481	B2	19840510		
IN 153525	A	19840721	IN 1980-CA783	19800705 <--
FR 2461715	A1	19810206	FR 1980-15682	19800716 <--
CA 1126750	A1	19820629	CA 1980-356655	19800721 <--
BR 8004564	A	19810203	BR 1980-4564	19800722 <--
JP 56022791	A2	19810303	JP 1980-99449	19800722 <--
JP 01008634	B4	19890214		
ES 493597	A1	19810616	ES 1980-493597	19800722 <--
ZA 8004419	A	19820224	ZA 1980-4419	19800722 <--

PRIORITY APPLN. INFO.: US 1979-59838 A 19790723

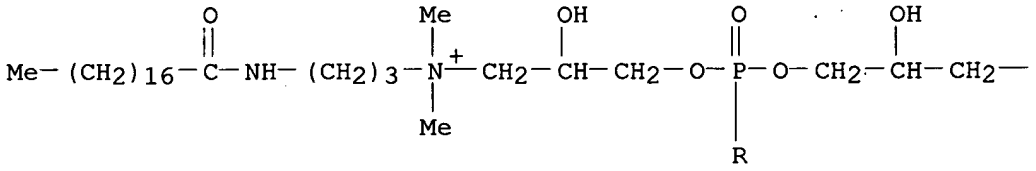
AB Title compds. were prepared for use in hair prepns. Thus, 19.0 g 85.5% H3PO4 were added dropwise to 46.53 g epichlorohydrin at 80-5°, the mixture was heated 1 h at 80°, 148 g C18H37NMe2 were added, and the mixture was heated 20 h at 102° to give OP[OCH2CH(OH)CH2NMe2C18H37]Cl 3, 98.6% pure.

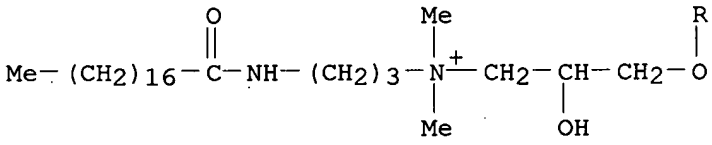
IT **75464-24-3P 77195-37-0P 77195-38-1P**
77195-39-2P 77583-79-0P 77583-80-3P
77593-31-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(manufacture of, for use in hair prepns.)

RN 75464-24-3 CAPLUS
CN 4,6-Dioxa-14-aza-10-azonia-5-phosphadotriacontan-1-aminium,

5-[3-[dimethyl[3-[(1-oxooctadecyl)amino]propyl]ammonio]-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-15-oxo-N-[3-[(1-oxooctadecyl)amino]propyl]-, trichloride, 5-oxide (9CI) (CA INDEX NAME)

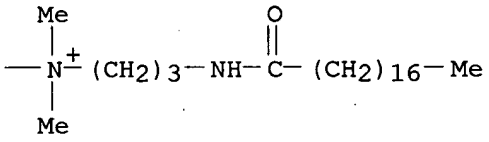
PAGE 1-A





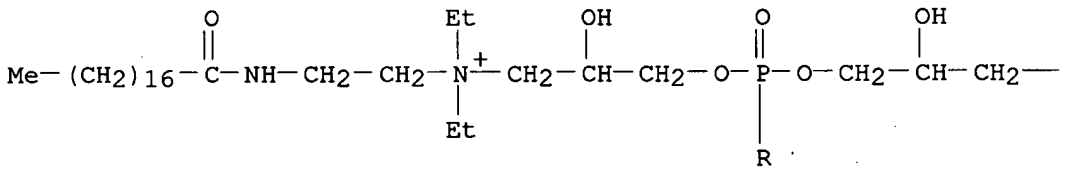
● 3 Cl^-

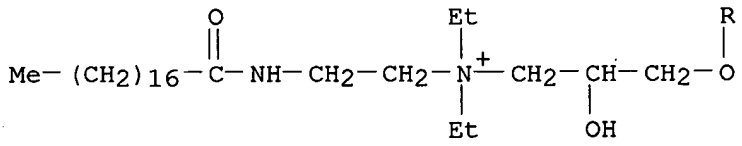
PAGE 1-B



RN 77195-37-0 CAPLUS
CN 4,6-Dioxa-13-aza-10-azonia-5-phosphahentriacontan-1-aminium, 5-[3-[diethyl[2-[(1-oxooctadecyl)amino]ethyl]ammonio]-2-hydroxypropoxy]-N,N,10,10-tetraethyl-2,8-dihydroxy-14-oxo-N-[2-[(1-oxooctadecyl)amino]ethyl]-, trichloride, 5-oxide (9CI) (CA INDEX NAME)

PAGE 1-A





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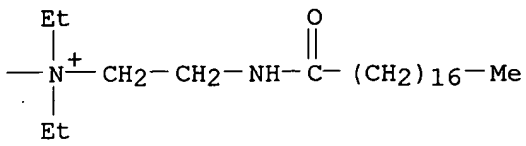
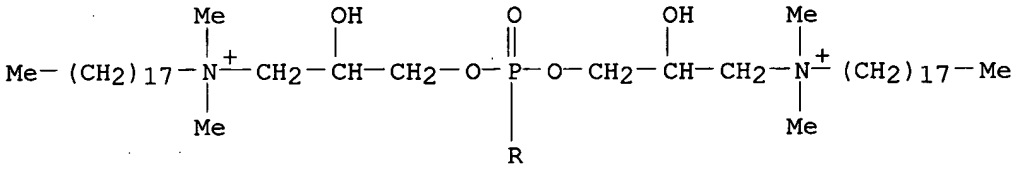
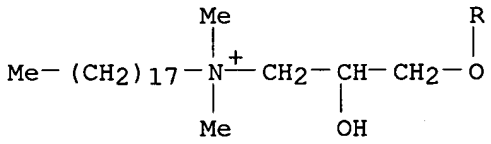


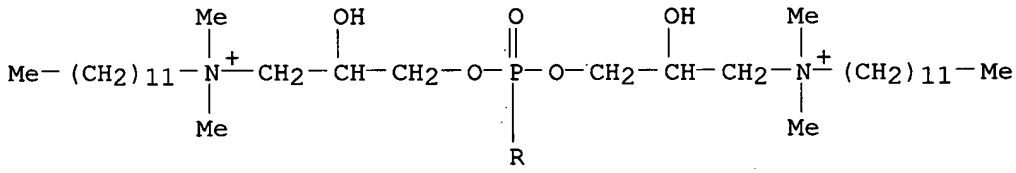
RN 77195-38-1 CAPLUS
CN 4,6-Dioxa-10-azonia-5-phosphaoctacosan-1-aminium, 5-[3-(dimethyloctadecylammonio)-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-N-octadecyl-, trichloride, 5-oxide (9CI) (CA INDEX NAME)

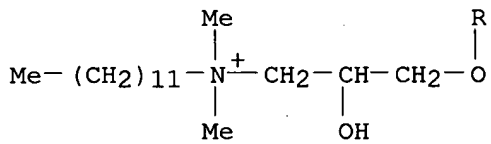




●3 Cl⁻

RN 77195-39-2 CAPLUS
CN 4,6-Dioxa-10-azonia-5-phosphadocosan-1-aminium, N-dodecyl-5-[3-(dodecyldimethylammonio)-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-, trichloride, 5-oxide (9CI) (CA INDEX NAME)

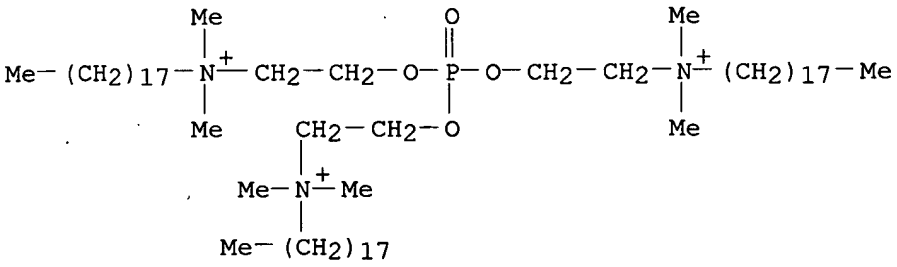




●3 Cl⁻

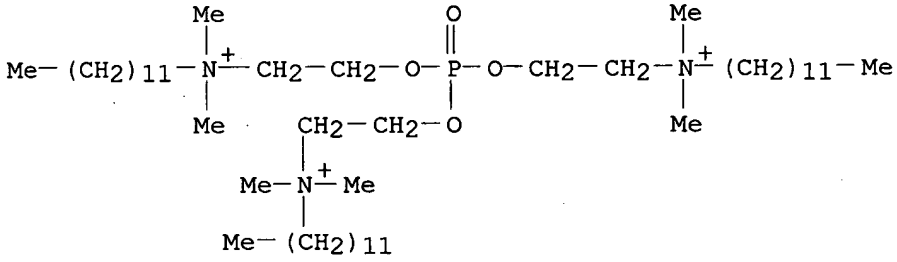
RN 77583-79-0 CAPLUS

CN 3,5-Dioxa-8-azonia-4-phosphahexacosan-1-aminium, 4-[2-(dimethyloctadecylammonio)ethoxy]-N,N,8,8-tetramethyl-N-octadecyl-, trichloride, 4-oxide (9CI) (CA INDEX NAME)



●3 Cl⁻

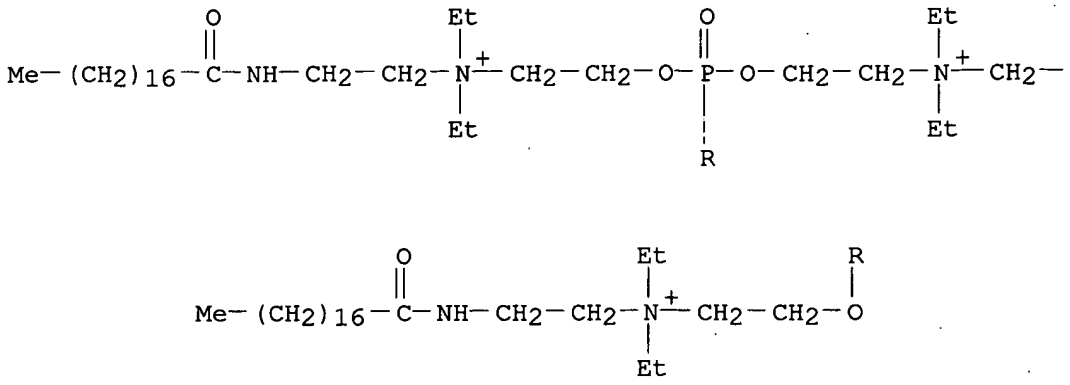
RN 77583-80-3 CAPLUS
CN 3,5-Dioxa-8-azonia-4-phosphaeicosan-1-aminium, N-dodecyl-4-[2-(dodecyldimethylammonio)ethoxy]-N,N,8,8-tetramethyl-, trichloride, 4-oxide (9CI) (CA INDEX NAME)



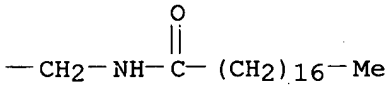
●3 Cl⁻

RN 77593-31-8 CAPLUS
CN 3,5-Dioxa-11-aza-8-azonia-4-phosphanonacosan-1-aminium, 4-[2-[diethyl[2-[(1-oxooctadecyl)amino]ethyl]ammonio]ethoxy]-N,N,8,8-tetraethyl-12-oxo-N-[2-[(1-oxooctadecyl)amino]ethyl]-, trichloride, 4-oxide (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L17 ANSWER 24 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1980:604049 CAPLUS
DOCUMENT NUMBER: 93:204049
TITLE: Phosphate **quaternary** compounds
INVENTOR(S): Mayhew, Raymond L.; O'Lenick, Anthony J.
PATENT ASSIGNEE(S): Mona Industries, Inc., USA
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4209449		19800624	US 1978-965458	19781130 <--

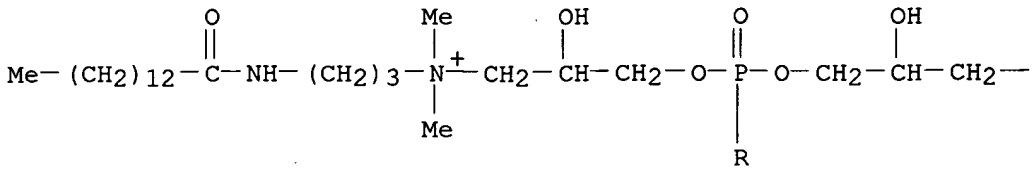
AB The **quaternary** compds. [R3N+CH2CH(OH)CH2O]3PO.3X- (R = alkyl, substituted alkyl, amidoalkyl; R3N = heterocyclic moiety; X = e.g., Cl), useful in detergents, cosmetics, wetting agents, etc., were prepared Thus, stirring [ClCH2CH(OH)CH2O]3PO with RCONH(CH2)3NMe2 (RCONH = cocamido) gave [RCONH(CH2)3N+Me2CH2CH(OH)CH2O]3PO.3Cl-.

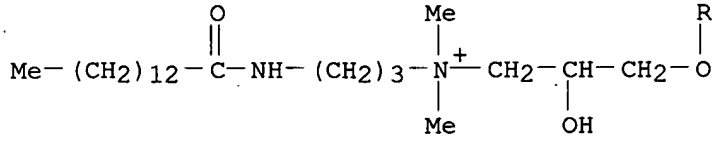
IT **75464-23-2P 75464-24-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and surfactant properties of)

RN 75464-23-2 CAPLUS

CN 4,6-Dioxa-14-aza-10-azonia-5-phosphaoctacosan-1-aminium, 5-[3-[dimethyl[3-[(1-oxotetradecyl)amino]propyl]ammonio]-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-15-oxo-N-[3-[(1-oxotetradecyl)amino]propyl]-, trichloride, 5-oxide (9CI) (CA INDEX NAME)

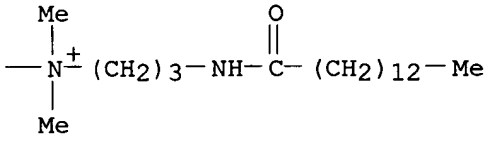
PAGE 1-A





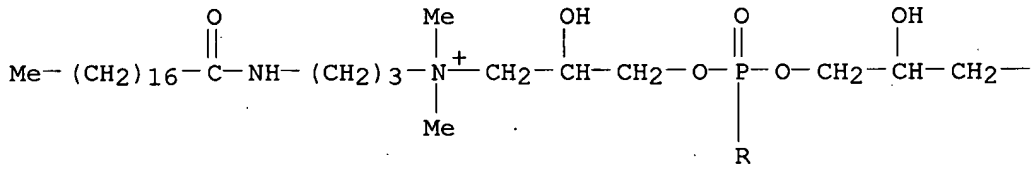
●3 Cl^-

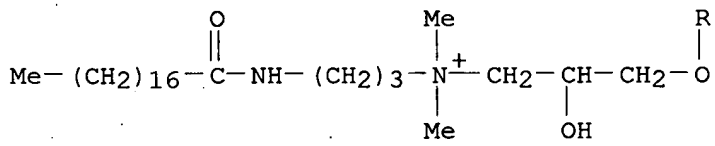
PAGE 1-B



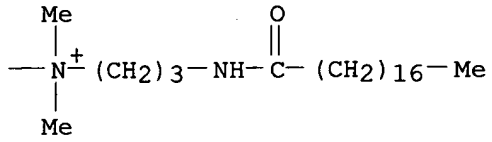
RN 75464-24-3 CAPLUS
CN 4,6-Dioxa-14-aza-10-azonia-5-phosphadotriacontan-1-aminium, 5-[3-[dimethyl[3-[(1-oxooctadecyl)amino]propyl]ammonio]-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-15-oxo-N-[3-[(1-oxooctadecyl)amino]propyl]-, trichloride, 5-oxide (9CI) (CA INDEX NAME)

PAGE 1-A





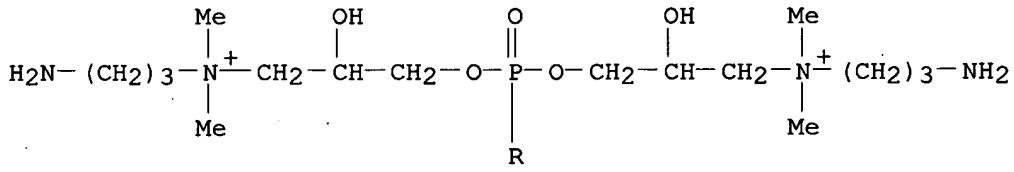
●3 Cl^-

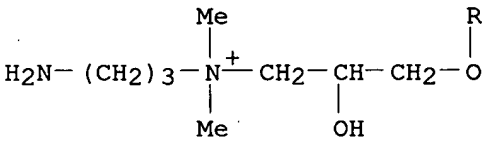


IT **75464-22-1DP**, N-cocoyl derivs. **75464-26-5P** **75464-27-6P** **75477-65-5P** **77195-39-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 75464-22-1 CAPLUS

CN 4,6-Dioxa-10-azonia-5-phosphatridecan-1-aminium, 13-amino-N-(3-aminopropyl)-5-[3-[(3-aminopropyl)dimethylammonio]-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-, trichloride, 5-oxide (9CI) (CA INDEX NAME)



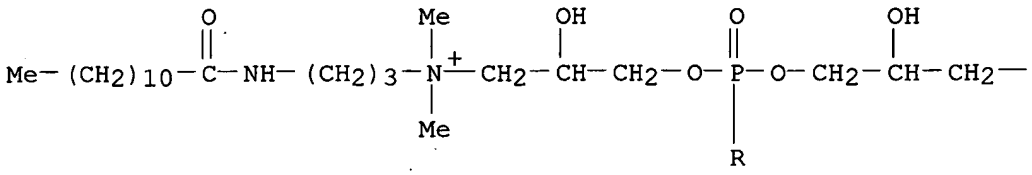


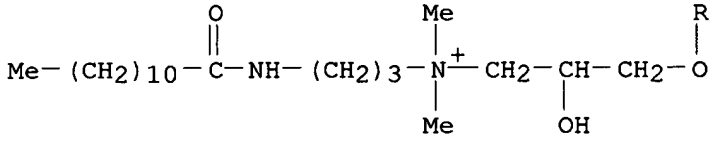
● 3 Cl^-

RN 75464-26-5 CAPLUS

CN 4,6-Dioxa-10-azonia-5-phosphatetracosan-1-aminium, 5-[3-(dimethyltetradecylammonio)-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-N-tetradecyl-, trichloride, 5-oxide (9CI) (CA INDEX NAME)

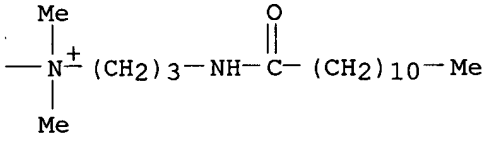
PAGE 1-A



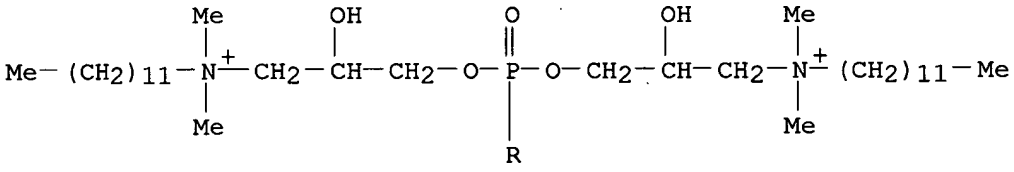


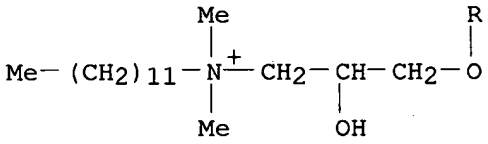
●3 Cl⁻

PAGE 1-B



RN 77195-39-2 CAPLUS
CN 4,6-Dioxa-10-azonia-5-phosphadocosan-1-aminium, N-dodecyl-5-[3-(dodecyldimethylammonio)-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-, trichloride, 5-oxide (9CI) (CA INDEX NAME)

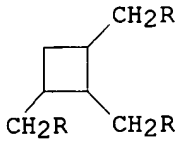




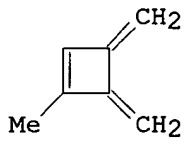
●3 Cl⁻

L17 ANSWER 25 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1980:75908 CAPLUS
DOCUMENT NUMBER: 92:75908
TITLE: Small rings. Part 31. Trimethylenecyclobutane
AUTHOR(S): Martin, Hans Dieter; Mayer, Bernhard

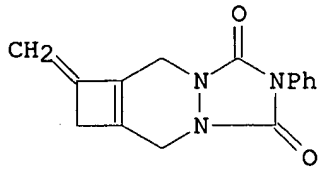
CORPORATE SOURCE: Inst. Org. Chem., Univ. Wuerzburg, Wuerzburg, D-8700, Fed. Rep. Ger.
SOURCE: Tetrahedron Letters (**1979**), (25), 2351-2
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 92:75908
GI



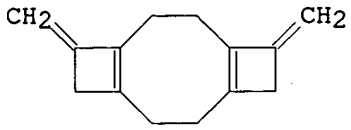
II



IV



V



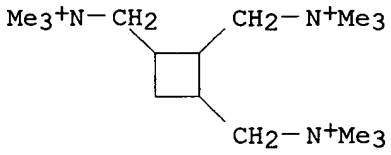
VI

AB The title compound (I) was prepared (60%) in 7 steps from EtO2CCH2CH2CBr2CO2Et, the key step being Cope elimination of the cyclobutane derivative II [R = N(O)Me2] (III). **Quaternization** of III with MeI gave II (R = N+Me3 OH-), which on thermolysis (80-130°) gave the cyclobutene derivative IV. I reacted with N-phenyl-1,2,4-triazoline-3,5-dione to give V and dimerized to give VI.

IT **72672-10-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermolysis of)

RN 72672-10-7 CAPLUS

CN 1,2,3-Cyclobutanetrimethanaminium, N,N,N,N',N',N',N'',N'',N''-nonamethyl-, trihydroxide (9CI) (CA INDEX NAME)



●3 OH⁻

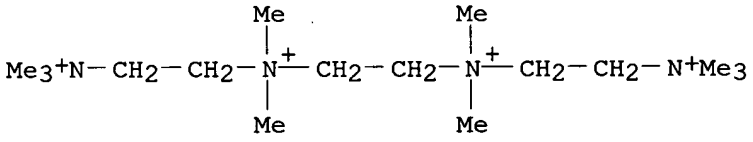
L17 ANSWER 26 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:585212 CAPLUS
DOCUMENT NUMBER: 87:185212
TITLE: Catalyses by polymer complexes. V. The heterotropic (allosteric) interaction of histamine- and hydroxamate-containing polymer catalysts with hydrophobic ammonium salts in the hydrolysis of phenyl esters
AUTHOR(S): Shinkai, Seiji; Tou, Kunio; Kunitake, Toyoki

CORPORATE SOURCE: Fac. Eng., Kyushu Univ., Fukuoka, Japan
SOURCE: Polymer Journal (Tokyo, Japan) (**1977**), 9(4), 381-9
CODEN: POLJB8; ISSN: 0032-3896
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Methacrylic acid-N-methacryloylhistamine copolymer (I) [64541-47-5], methacrylamide-N-methacryloylhistamine copolymer [64541-48-6] and methacrylic acid-methacrylohydroxamic acid copolymer (II) [64541-49-7] were prepared and their hydrolytic reactivities toward p-nitrophenyl acetate (III) [830-03-5] and p-nitrophenyl hexanoate (IV) [956-75-2] were studied in the absence and in the presence of hydrophobic ammonium salts. The nucleophilic reactivity of I toward III was hardly affected by the addition of hydrophobic ammonium ions, while a marked increase of rates was found in the reaction with IV. Addition of these ammonium ions to the II system enhanced the rate of reaction with IV by lowering the pKa (0.3-0.4 pK unit) and by increasing the second-order rate constant (.apprx.3-fold), as inferred from the pH-rate profile. The rate-enhancing effect of the hydrophobic ammonium salts was analyzed by using the Hill equation which has been employed for analyzing allosteric behavior in enzyme systems; the observed coefficient (n = 3-4) suggested that polymer-bound ammonium ions facilitated the subsequent binding.

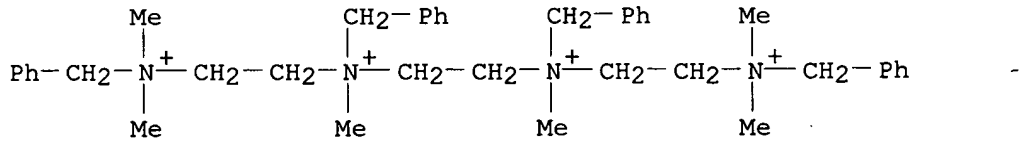
IT **64554-59-2 64554-60-5 64554-61-6**
64596-41-4 64596-42-5
RL: PRP (Properties)
(heterotropic interaction of, with histamine- and hydroxamate-containing polymer catalysts, in hydrolysis of phenyl esters)

RN 64554-59-2 CAPLUS
CN 1,2-Ethanediaminium, N,N,N',N'-tetramethyl-N,N'-bis[2-(trimethylammonio)ethyl]-, tetrabromide (9CI) (CA INDEX NAME)



●4 Br^-

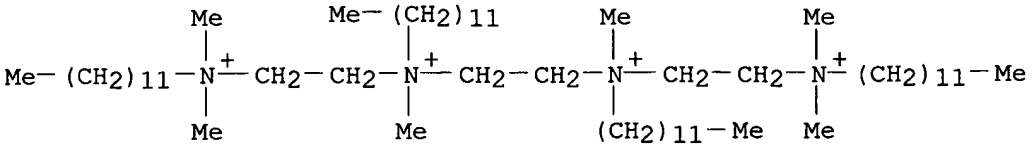
RN 64554-60-5 CAPLUS
CN 1,2-Ethanediaminium, N,N'-bis[2-[dimethyl(phenylmethyl)ammonio]-N,N'-dimethyl-N,N'-bis(phenylmethyl)-, tetrabromide (9CI) (CA INDEX NAME)



●4 Br^-

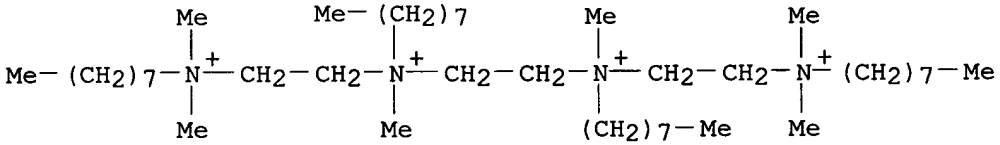
RN 64554-61-6 CAPLUS
CN 1,2-Ethanediaminium, N,N'-didodecyl-N,N'-bis[2-(dodecyldimethylammonio)ethyl]-N,N'-dimethyl-, tetrabromide (9CI) (CA

INDEX NAME)



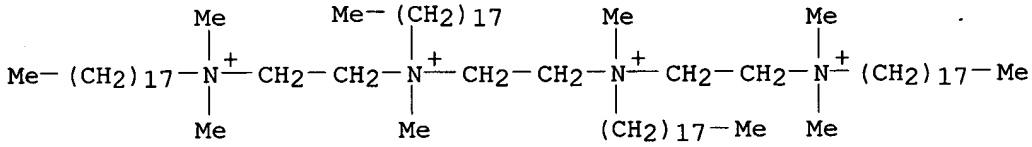
● 4 Br^-

RN 64596-41-4 CAPLUS
CN 1,2-Ethanediaminium, N,N'-bis[2-(dimethyloctylammonio)ethyl]-N,N'-dimethyl-N,N'-dioctyl-, tetrabromide (9CI) (CA INDEX NAME)



● 4 Br^-

RN 64596-42-5 CAPLUS
CN 1,2-Ethanediaminium, N,N'-bis[2-(dimethyloctadecylammonio)ethyl]-N,N'-dimethyl-N,N'-dioctadecyl-, tetrabromide (9CI) (CA INDEX NAME)



● 4 Br^-

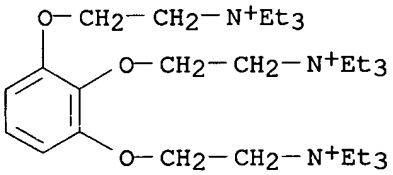
L17 ANSWER 27 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1975:589843 CAPLUS
DOCUMENT NUMBER: 83:189843
TITLE: Reactivation and aging of diphenyl phosphoryl acetylcholinesterase
AUTHOR(S): Maglothin, James A.; Wins, Pierre; Wilson, Irwin B.
CORPORATE SOURCE: Dep. Chem., Univ. Colorado, Boulder, CO, USA
SOURCE: Biochimica et Biophysica Acta (**1975**), 403(2), 370-87
CODEN: BBACAQ; ISSN: 0006-3002
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Acetylcholinesterase (EC 3.1.1.7) was readily inhibited by 10-5M diphenylphosphorochloridate even though the inhibitor hydrolyzes in a few seconds. The fluoridate was a much weaker inhibitor. The inhibited enzyme, diphenylphosphoryl enzyme spontaneously recovered only .apprx.50% of its activity with a half time of .apprx.17 min at pH 7.0 and 6 min at pH 8.0. The fact that only 50% of the original activity returns was due to aging. The rates of reactivation and aging were very greatly increased by a few percent of an organic solvent. Depending on the solvent, even 1% may increase the rates by a factor of 5-6. The highest increase in rate was 70-fold. **Quaternary** NH4+ also increased the rates. Organic solvents and NH4+ also accelerated the reactivation of the much more stable diethylphosphoryl enzyme derivative

IT **65-29-2**
RL: BIOL (Biological study)
(aging and reactivation of diphenylphosphoryl acetylcholinesterase response to)

RN 65-29-2 CAPLUS

CN Ethanaminium, 2,2',2''-[1,2,3-benzenetriyltris(oxy)]tris[N,N,N-triethyl-, triiodide (9CI) (CA INDEX NAME)



●3 I^-

L17 ANSWER 28 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1964:34024 CAPLUS

DOCUMENT NUMBER: 60:34024

ORIGINAL REFERENCE NO.: 60:6087d-e

TITLE: The excitation of lateral geniculate neurons by **quaternary** ammonium derivatives

AUTHOR(S): Curtis, D. R.; Davis, R.

CORPORATE SOURCE: Australian Natl. Univ., Canberra

SOURCE: Journal of Physiology (Cambridge, United Kingdom) (**1963**), 165(1), 62-82
CODEN: JPHYA7; ISSN: 0022-3751

DOCUMENT TYPE: Journal

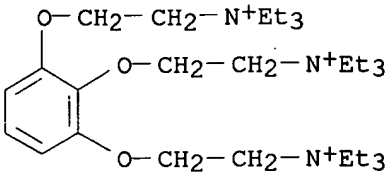
LANGUAGE: Unavailable

AB Carbamoylcholine was the most active excitant tested on cat neurons. Synaptic excitation by the optic nerve, but not by acetylcholine, was suppressed by 5-hydroxytryptamine; dihydro-β-erythroidine had the inverse effect.

IT **65-29-2**, [v-Phenenyltris(oxyethylene)]tris[triethylammonium iodide]
(nerve response to)

RN 65-29-2 CAPLUS

CN Ethanaminium, 2,2',2''-[1,2,3-benzenetriyltris(oxy)]tris[N,N,N-triethyl-, triiodide (9CI) (CA INDEX NAME)



●3 I^-

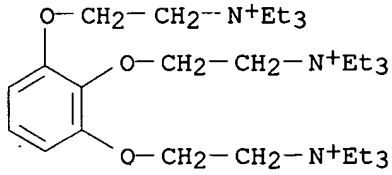
L17 ANSWER 29 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1963:434890 CAPLUS
DOCUMENT NUMBER: 59:34890
ORIGINAL REFERENCE NO.: 59:6196e-f
TITLE: The use of paper chromatographic methods for the toxicological determination of drugs. III. Paper chromatographic behavior of several basic drugs as affected by their structure
AUTHOR(S): Vecerkova, J.; Solc, J.; Kacl, K.
CORPORATE SOURCE: Karlova Univ., Prague
SOURCE: Journal of Chromatography (**1963**), 10, 479-92
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: German

AB cf. CA 58, 2326b, 3714f. The relation between the structure and paper chromatographic behavior of 30 basic drugs was studied, using the reverse phase system petroleum (b.p. 195-220°)-EtOH-H2ONH3, in which the proportions of EtOH and H2O were varied 7 times. In all cases except 3, Rf increased with increasing EtOH content for 20 tertiary bases and decreased for 10 **quaternary** bases. For most compds., the Rf was lower at 12-13° than at 17°. Rf values in the 7 solvent systems are tabulated for all compds.

IT **65-29-2**, [v-Phenenyltris(oxyethylene)]tris[triethylammonium iodide]
(chromatography of)

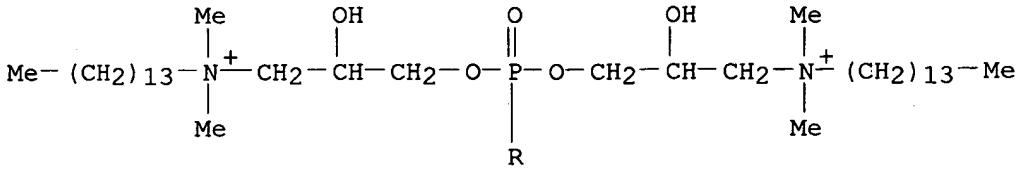
RN 65-29-2 CAPLUS

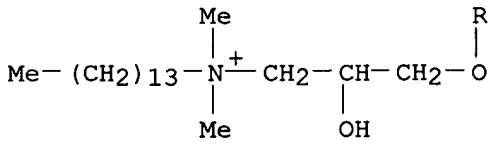
CN Ethanaminium, 2,2',2''-[1,2,3-benzenetriyltris(oxy)]tris[N,N,N-triethyl-, triiodide (9CI) (CA INDEX NAME)



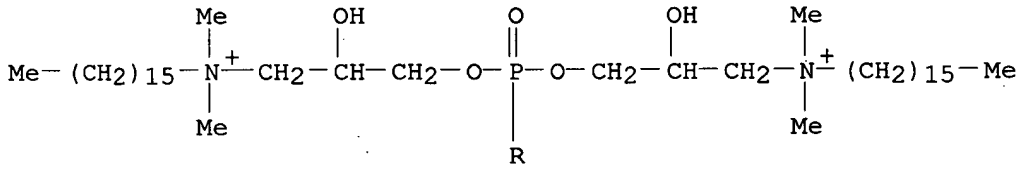
●3 I^-

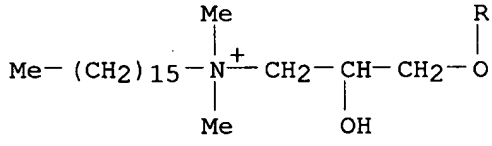
L17 ANSWER 30 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1963:415185 CAPLUS
DOCUMENT NUMBER: 59:15185
ORIGINAL REFERENCE NO.: 59:2657c-d





RN 75464-27-6 CAPLUS
CN 4,6-Dioxa-10-azonia-5-phosphahexacosan-1-aminium, N-hexadecyl-5-[3-(hexadecyldimethylammonio)-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-, trichloride, 5-oxide (9CI) (CA INDEX NAME)





RN 75477-65-5 CAPLUS
CN 4,6-Dioxa-14-aza-10-azonia-5-phosphahexacosan-1-aminium, 5-[3-[dimethyl[3-[(1-oxododecyl)amino]propyl]ammonio]-2-hydroxypropoxy]-2,8-dihydroxy-N,N,10,10-tetramethyl-15-oxo-N-[3-[(1-oxododecyl)amino]propyl]-, trichloride, 5-oxide (9CI) (CA INDEX NAME)

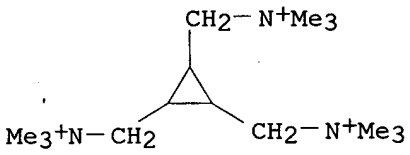
TITLE: Cyclopropane methonium compounds
AUTHOR(S): Burger, Alfred; Bedford, G. R.
CORPORATE SOURCE: Univ. of Virginia, Charlottesville
SOURCE: Journal of Medicinal Chemistry (**1963**), 6(4), 402-5
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB In a study of the effect of limiting the flexibility of the chains of methonium compds. on the pharmacol. actions of certain stereoisomers, analogs of hexamethonium and succinylcholine carrying a cis or trans oriented cyclopropane ring in the center of the chain were synthesized. The geometric isomers of bis(trimethylammoniumethyl) cyclopropane-1,2-dicarboxylate and of the homologous cyclopropane-1,2-diacetate **ester** diiodides caused predominantly neuromuscular block and resembled succinylcholine. The geometric isomers of 1,2-bis(β-trimethylammoniumethyl)cyclopropane diiodide exerted primarily ganglionic blockade of the hexamethonium type. The trans isomer was the more potent in each case.

IT **97299-16-6**, Ammonium, [1,2,3-cyclopropanetriyltris(methylene)]tris[trimethyl-iodide]
(cyclopropyl derivs.)

RN 97299-16-6 CAPLUS

CN [1,2,3-Cyclopropanetriyltris(methylene)]tris[trimethylammonium iodide] (7CI) (CA INDEX NAME)



●3 I⁻

=> d l17 31-43 ibib abs hitstr

L17 ANSWER 31 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1962:479123 CAPLUS
DOCUMENT NUMBER: 57:79123
ORIGINAL REFERENCE NO.: 57:15747d-e
TITLE: Neuromuscular-blocking agents. IX. Short-acting linear N,N,N-trisonium esters
AUTHOR(S): Carey Macleod, Fiona; Lewis, J. J.; Stenlake, J. B.; Williams, W. D.
CORPORATE SOURCE: Univ. Glasgow, UK
SOURCE: Journal of Pharmacy and Pharmacology (**1961**), 13(Suppl.), 103T-106T
CODEN: JPPMAB; ISSN: 0022-3573
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

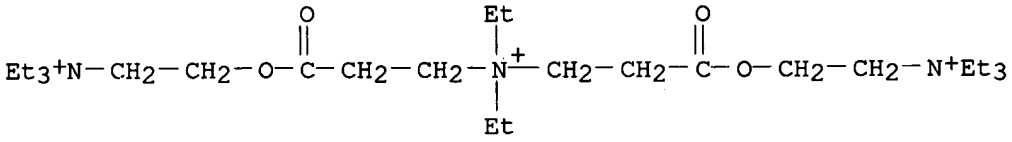
AB cf. CA 54, 11981c; 56, 7932c. The short series of linear trisonium esters are synthesized and are compared with tubocurarine, and suxamethonium for neuromuscular-blocking properties, potency, and toxicity. All compds. synthesized are tubocurarine-like except the methonium derivative (I), which is a depolarizing agent. I (3.0 mg./kg.) causes an inhibition of

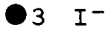
contractions and the development of contracture in the gastrocnemins musclesciatic nerve preparation of the pentobarbitone-anesthetized hen. Similar effects are obtained with 0.05 mg./kg. suxamethonium chloride.

IT **17089-56-4**, Ammonium, bis(2-carboxyethyl)diethyl, iodide, diester with triethyl(2-hydroxyethyl)ammonium iodide **17089-57-5**, Choline, iodide, diester with bis(2-carboxyethyl)ethylmethylammonium iodide
(nerve-muscle transmission blocking by)

RN 17089-56-4 CAPLUS

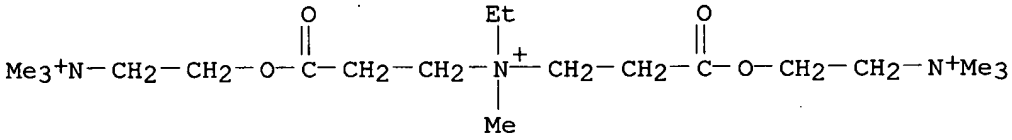
CN 1-Propanaminium, N,N-diethyl-3-oxo-N-[3-oxo-3-[2-(triethylammonio)ethoxy]propyl]-3-[2-(triethylammonio)ethoxy]-, triiodide (9CI) (CA INDEX NAME)

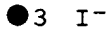




RN 17089-57-5 CAPLUS

CN 1-Propanaminium, N-ethyl-N-methyl-3-oxo-N-[3-oxo-3-[2-(trimethylammonio)ethoxy]propyl]-3-[2-(trimethylammonio)ethoxy]-, triiodide (9CI) (CA INDEX NAME)





L17 ANSWER 32 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1961:143790 CAPLUS

DOCUMENT NUMBER: 55:143790

ORIGINAL REFERENCE NO.: 55:27155e-i,27156a-i

TITLE: New class of local anesthetics. Hydroxyalkyliminobisacetamides

AUTHOR(S): Freed, Meier E.; Bruce, William F.; Hanslick, Roy S.; Maschitti, Albert

CORPORATE SOURCE: Wyeth Labs., Philadelphia, PA

SOURCE: Journal of Organic Chemistry (**1961**), 26, 2378-83
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. CA 53, 6088e. A series of hydroxyalkyliminobisacetamides, HOXN(CH2CONRR1)CH2CONR2R3 (where X is alkylene, cycloalkylene, or aralkylene, R, R1, R2, R3 represent lower alkyl or aralkyl, and where RR1 may or may not equal R2R3), were prepared, examined for local anesthetic action, and studied for structure-activity relationships. The preparation of

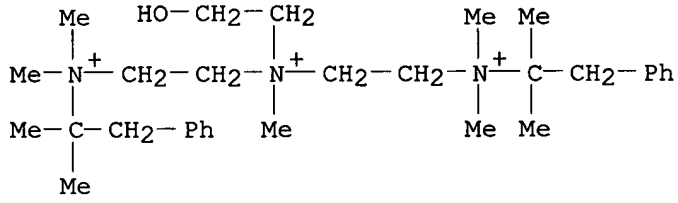
all chloroacetamides, hydroxyalkylaminoacetamides, hydroxyalkyliminoacetamides and their esters were carried out essentially in the same manner. PhCH2CMe2NHMe (0.86 mole) in 500 ml. PhMe stirred 1 hr. at -15° with addition of 0.40 mole ClCH2COCl, the mixture filtered at 20°, the amine HCl salt washed with PhMe, the combined filtrate and washings dried, and the residue on evaporation distilled yielded 70.5% PhCH2CMe2NMeCOCH2Cl (I), b0.5 140-1°. HOCH2CH2 NH2 (0.1 mole) and 30 g. anhydrous powdered Na2CO3 in 300 ml. well-stirred boiling BuOH slowly treated with 0.1 mole I in 50 ml. BuOH, the mixture refluxed 12 hrs., cooled, and filtered, and the residue on evaporation crystallized from C6H14 yielded 63% HOCH2CH2NHCH2CONMeCMe2CH2Ph, m. 74.5-6.5°; HCl salt, m. 163-4°. Similarly were prepared and tabulated hydroxyalkylaminoacetamides, RNHCH2CONR1Me (R, R1, and m.p. HCl salt given): PhCHOHCH2, PhCH2CMe2, 201-2°; PhCHOHCMe2, PhCH2CMe2, 189-90°; HOCH2CMe2, PhCH2CMe2, 169-70°; (HOCH2)3C, PhCH2CMe2, 175-6°; HOCHMeCH2, PhCH2, 134-5°. I (0.1 mole) and 20 g. K2CO3 in 250 ml. boiling BuOH stirred with addition of 0.05 mole freshly distilled HOCH2CH2NH2, the mixture refluxed 20 hrs. and the cooled mixture filtered, the filtrate washed (aqueous 5% Na2CO3, H2O) and the dried (MgSO4) solution evaporated in vacuo yielded 71% hydroxyalkyliminobisacetamide, RN(CH2CONR1R2)2 (II) (R = HOCH2CH2, R1 = Me, R2 = PhCH2CMe2) (III), m. 104-5°; HCl salt m. 146-7° (MeOH-Me2CO); nicotinic acid **ester** m. 158-9°. III (20 g.) in 100 ml. dry CHCl3 treated with 5 g. SOCl2 in 25 ml. CHCl3, the mixture stirred 3 hrs., and the residue on evaporation crystallized from alc.-Et2O yielded 79 g. II (R = ClCH2CH2, R1 = Me, R2 = PhCH2CMe2) HCl salt (IV), m. 155-6° (alc.-Et2O). IV (3 g.) in 20 ml. MeOH containing 3 g. anhydrous NH3 heated 18 hrs. at 90° in a pressure tube, the cooled mixture and MeOH rinsings filtered from NH4Cl, freed from MeOH and excess NH3, and taken up in 50 ml. Me2CHOH, and the filtered solution treated with dry HCl and diluted with 150 ml. dry Et2O yielded 40.5% II (R = H2NCH2CH2, R1 = Me, R2 = PhCH2CMe2), m. 231-2°. III (0.02 mole) in 150 ml. dry Et2O added slowly with stirring to 1.8 g. LiAlH4 in 300 ml. dry Et2O, the mixture refluxed 25 hrs. before cautious decomposition with 8 ml. H2O, the dried Et2O layer treated with HCl, the oily product triturated with Me2CO, and the product (29.3%) recrystd. from MeOHMe2CO yielded HOCH2CH2N(CH2CH2NMeCMe2CH2Ph)2, m. 229-30° (decomposition); tri-HCl salt m. 239-40°; MeI salt, m. 122-3°; tri-MeI salt, m. 154-5°. To obtain the bis compds. with sterically hindered amino alcs., the use of a higher boiling solvent (such as PhOMe) was necessary. Phys. and pharmacol. data are tabulated for the various series of compds., RN(CH2CONR1R2)2 (R, R1, R2, b.p./mm., duration of activity on rabbit cornea and % solution given): HOCH2CH2, (R1R2=)CH2CH2, 203-5°/1.0, neg., 0.1; HOCH2CH2, Me(CH2)3, Me(CH2)3, 208-10°/0.5, 25 min., 0.01; MeCHOHCH2, Me(CH2)3, Me(CH2)3, 200-5°/0.1, neg., 0.1; HOCH2CH2, Me2CHCH2, Me2CHCH2, 170-1°/0.5, neg., 0.1; HO(CH2)3, Me2CHCH2, Me2CHCH2, 190-2°/0.5, neg., 0.1; HOCH2CMe2, Me(CH2)3, Me(CH2)3, 155-60°/0.5, neg., 0.1; HOCH2CMe2, MeCH2, Me(CH2)3, 170-5°/0.5, neg., 0.1; HO(CH2)22, Me(CH2)4, Me(CH2)4, 230-5°/1.0, neg., 0.1; HO(CH2)2, C6H11, C6H11, - (HCl salt m. 215-16°), neg., 0.1; HO(CH2)2, Me(CH2)5, Me(CH2)5, 194-6°/0.5, 48 min., 0.1. For RN(CH2CONR1R2)2 [R, R1, R2, m.p. of base or HCl salt (or b.p./mm.), duration in min. and % solution given): HO(CH2)2, Me, PhCH2CMe2, 104-4.5°, 25, 0.0005; HOCHMeCH2, Me, PhCH2CMe2, 113-14°, 28, 0.0001; HOCH2CHEt, Me, PhCH2CMe2, 144-5° (HCl salt), 37, 0.0005; HO(CH2)3, Me, PhCH2CMe2, 164-5° (HCl salt), 82, 0.1; HO(CH2)6, Me, PhCH2CMe2, 250-60°/0.002, neg., 0.1; (HOCH2)3C, Me, PhCH2CMe2, 157-8°, 24, 0.001; 2-HOC6H10, Me, PhCH2CMe2, 108.0-8.5°, 75, 0.0025; PhCHOHCH2, Me, PhCH2CMe2, 182-3° (HCl salt), 24, 0.001; PhCHOHCMe2,

Me, PhCH2CMe2, 203-4° (HCl salt), neg., 0.1; HO(CH2)2, Me, C6H11, 190-5°/1.0, neg., 0.1; HO(CH2)2, H, PhCH2CH2, 72-3° (HCl salt), neg., 0.1; HO(CH2)2, Me(CH2)3, PhCH2, 118° (HCl salt), 29, 0.001; HOCHMeCH2, Me(CH2)5, PhCH2, 195-200°/0.05, 44, 0.1; HOCHMeCH2, H, 2,6-Me2C6H3, 193-4° (HCl salt), neg. 0.1. For RN(CH2CONR1R2)CH2CONR3R4 (R, R1, R2, R3, R4, b.p./mm, or m.p. of base or HCl salt, duration, and % solution given): HO(CH2)2, MeCH2, MeCH2, Me(CH2)3, Me(CH2)3, 203-5°/1.0, 29. 0.1; HO(CH2)2, Me(CH2)2, Me(CH2)2, Me(CH2))3, Me2CHCH2, 198-200°/0.5, 21, 0.1; HO(CH2)2, MeCH2, MeCH2, Me, PhCH2CMe2, 121-2°, neg., 0.1; HO(CH2)2, Me(CH2)4, Me(CH2)4, Me, PhCH2CMe2, 92-3°, 63, 0.1; HO(CH2)3, Me2CHCH2, Me2CHCH2, Me, C6H11, 205-80/1.0, neg., 0.1; HO(CH2)2, Me, PhCH2CHMe, Me, PhCH2CMe2, hygroscopic, 55, 0.001; HO(CH2)2, H, PhCH2CH2, Me, PhCH2CMe2, 158° (HCl salt), neg., 0.1; HO(CH2)2, H, HOCH2CH2, Me, PhCH2CMe2, 42° (HCl salt), neg., 0.1; HO(CH2)2, H, Me(CH2)5, Me, PhCH2CMe2, 260°/1.0, 9, 0.05. For XCH2CH2N(CH2CONR1R2)2 (X, R1, R2, m.p. HCl salt, duration, and % solution): MeCO2, Me, PhCH2CMe2, 169-70°, 32, 0.001; Me(CH2)10CO2, Me, PhCH2CMe2, 143-5°, 38, 0.01; p-MeC6H4CO2, Me, PhCH2CMe2, 168-9°, 42, 0.001; p-O2NC6H4CO2, Me, PhCH2CMe2, 168-9°, 27, 0.0005; MeCO2, Me(CH2)3, Me(CH2)3, 212-14°/0.05(base), 32, 0.01; m-ClC6H4CO2, Me, PhCH2CMe2, 87-8° (base, from Me2CHOH-petr. ether), active, 0.1; (3-C5H4N)CO2, Me, PhCH2CMe2, 158-9°, 35, 0.0005; p-MeOC6H4CO2, Me, PhCH2CMe2, 126-7°, active, 0.1; p-H2NC6H4CO2, Me, PhCH2CMe2, 199-200°, active, 0.1. Iminoacetamides in which the amido N was derived from aliphatic amines had relatively little local anesthetic action and were more toxic than those derived from aralkyl amines. The use of PhCH2CMe2NHMe produced the highest degree of local anesthetic activity in II. Substitution of PhCH2CHMeNHMe in 1 **amide** group halved the activity. In the alkanolamine moiety, use of a sterically hindered base (H2NCMe2CH2OH) markedly reduced activity. Separation of HO from the tertiary amino group by interposition of CH2 groups reduced activity. The activity of HOCH2CH2CH2N(CH2CONMeCMe2CH2Ph)2 was 1/500 of that of the homologous HOCH2CH2N(CH2CONMeCMe2CH2Ph)2. Replacement of HO by NH2 or Cl, and **quaternization** of the tertiary amine or reduction of the **amide** groups to tertiary amines all resulted in nearly complete loss of activity. The activity was not increased by **ester** formation.

IT **119722-18-8**, Ammonium, [(2 hydroxyethylimino)diethylene]bis[(.alpha.,α-dimethylphenethyl)dimethyl- iodide], methiodide
(preparation of)

RN 119722-18-8 CAPLUS

CN [(2-Hydroxyethylimino)diethylene]bis[(α,α-dimethylphenethyl)dimethylammonium iodide] methiodide (6CI) (CA INDEX NAME)



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L17 ANSWER 33 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1960:126132 CAPLUS

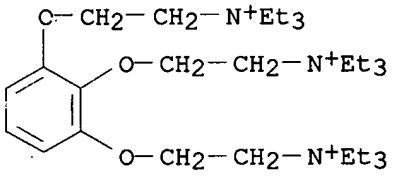
DOCUMENT NUMBER: 54:126132
ORIGINAL REFERENCE NO.: 54:24016f-g
TITLE: Action of some **quaternary** ammonium salts with curare-like effect on the polarographic behavior of cystine
AUTHOR(S): Serban, Mihail
SOURCE: Acad. rep. populare Romine, Inst. biochim., Studii cercetari biochim. (**1958**), 1, 369-79
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB The action of d-turocurarine, flaxedyl, decamethonium, succinylcholine, and "C100" on the polarog. wave of cystine was studied. All of these substances increased the catalytic current, i.e. the height of the cystine wave, the magnitude of the effect depending on the concentration of the salts.

IT **65-29-2**, Ammonium, [v-phenenyltris(oxyethylene)]tris[triethyl-iodide]
(cystine polarog. in presence of)

RN 65-29-2 CAPLUS

CN Ethanaminium, 2,2',2''-[1,2,3-benzenetriyltris(oxy)]tris[N,N,N-triethyl-, triiodide (9CI) (CA INDEX NAME)



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L17 ANSWER 34 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1960:62276 CAPLUS
DOCUMENT NUMBER: 54:62276
ORIGINAL REFERENCE NO.: 54:11981c-h
TITLE: Neuromuscular blocking agents. IV. Synthesis and study of N- and S-alkyl variants of dihexasulfonium and dihexazonium triethiodides
AUTHOR(S): Carey, Fiona M.; Edwards, D.; Lewis, J. J.; Stenlake, J. B.
SOURCE: Journal of Pharmacy and Pharmacology (**1959**), 11, Suppl. 70T-86T
CODEN: JPPMAB; ISSN: 0022-3573
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

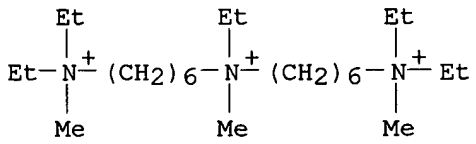
AB cf. C.A. 53, 9032c. N,S,N- and N,N,N-Tri onium compds., related to dihexasulfonium and dihexazonium in which N-alkyl substituents were varied, were prepared N,S,N-Trionium compds. were prepared from either bis(6-dimethylaminohexyl)sulfide or bis(6-diethylaminohexyl)sulfide by refluxing with the alkyl halide in EtOH, evaporating, and crystallizing Compds. with
min. of reflux, % yield, m.p., and crystallization solvent were: 7-ethyl-7-thioniatridecylenebis(dimethylammonium) triiodide, 35, 61, 137-7.5°, EtOH; 7-butyl-7-thioniatridecylenebis(dimethylbutylammoni um) triiodide, 40, 51, 131-1.5°, EtOH-Me2COEt2O; 7-methyl-7-thioniatridecylenebis(diethylmethylammonium) triiodide, 20, 94, 135-6°, EtOH; 7-propyl-7-thioniatridecylenebis(diethylpropylammoniu

m) triiodide, 45, 52, 125.5-26°, EtOH-Et2O. Et N,N-dipropyladipamate (from Et H adipate), yellow oil, b0.35 144-6°, nD22 1.4550, 87.6%. 6-Hydroxyhexyldipropylamine (from N,N-dipropyladipate by LiAlH4) b0.65 115-17°, nD22 1.4533, 95%. 6-Propylaminohexyldipropylamine (from reflux of 6 - hydroxyhexyldipropylamine and HBr, then propylamine), b0.45 115-17°, nD22, 1.4463, 70.6%. N,N-Dipropyladipamic acid (by hydrolysis of Et N,N-dipropyladipamate in alc. KOH), yellow viscous oil, b0.5 198°, nD25 1.4723, 91.9%. Bis(6-dipropylaminohexyl)propylamin e (from reflux of N,N-dipropyladipamic acid in C6H6 and SOCl2), pale yellow oil, b0.65 211°, nD21 1.4582, 77.5%. N,N-Diethyladipamic acid, yellow viscous oil, b0.5 182°, nD20.5 1.4733, 95.7%. Bis(6-diethylaminohexyl)ethylamine (from N,N-diethyladipamic acid and excess 6-(diethylaminohexyl)ethylamine), pale yellow oil, b0.75 173-6°, nD25 1.4588, 55.9%. N,N,N-Trionium compds., prepared from either bis(6-dipropylaminohexyl)propylamine or bis(6-diethylaminohexyl)ethylamine by reflux with alkyl halide in EtOH, evaporation, and crystallization, were (min. of reflux, % yield, m.p., and solvent given): 7-methyl-7-propyl-7-azoniatridecylenebis(dipropylmethylammonium) triiodide, 10, 94, 239°, EtOH; 7-ethyl-7-propyl-7-azoniatridecylenebis(dipropylethylammonium) triiodide, 35, 66, 221°, EtOH-Me2O-Et2O; 7,7-dipropyl-7-azoniatridecylenebis(tripropyl ammonium) triiodide, 45, 12, 206-7°, Me2COEt2O; 7-ethyl-7-methyl-7-azoniatridecylenebis(diethylmethylammonium) triiodide, 5, 88, 227.5-8.5°, MeOH; 7-ethyl-7-propyl-7-azoniatridecylenebis(diethylpropylammonium) triiodide, 30, 43, 220°, EtOH-Me2CO-Et2O; 7-ethyl-7-butyl-7-azoniatridecylenebis(diethylpropylaminonium) triiodide, 45, 61, 178°, Me2CO-Et2O. All the compds. tested qual. resembled tubocurarine in their action. Stepwise replacement of Et by Me in dihexasulfonium triethiodide (I) decreased potency. Potency also fell when Et groups were replaced by Pr in I and dihexazonium triethiodide.

IT **1862-35-7**, Ammonium, [(ethylimino)bis(hexamethylene)]bis[diethyl methyl- iodide], methiodide **1862-36-8**, Ammonium, [(propylimino)bis(hexamethylene)]bis[diethylpropyl- iodide], ethiodide **1862-37-9**, Ammonium, [(propylimino)bis(hexamethylene)]bis[ethyldip ropyl- iodide], ethiodide **1862-38-0**, Ammonium, [(propylimino)bis(hexamethylene)]bis[tripropyl- iodide], propiodide **4055-56-5**, Ammonium, [(propylimino)bis(hexamethylene)]bis[methyldi propyl- iodide], methiodide **124245-58-5**, Ammonium, [(butylimino)bis(hexamethylene)]bis[diethylpropyl- iodide]-, ethiodide (preparation of)

RN 1862-35-7 CAPLUS

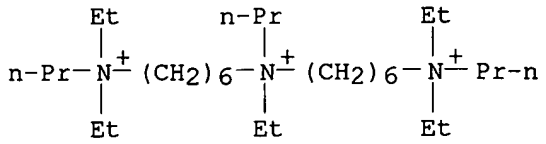
CN 1,6-Hexanediaminium, N-[6-(diethylmethylammonio)hexyl]-N,N',N'-triethyl-N,N'-dimethyl-, triiodide (9CI) (CA INDEX NAME)



●3 I⁻

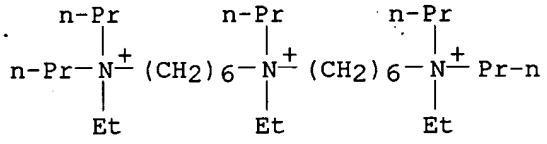
RN 1862-36-8 CAPLUS

CN 1,6-Hexanediaminium, N-[6-(diethylpropylammonio)hexyl]-N,N',N'-triethyl-N,N'-dipropyl-, triiodide (9CI) (CA INDEX NAME)



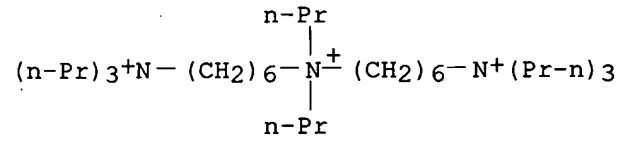
●3 I^-

RN 1862-37-9 CAPLUS
CN 1,6-Hexanediaminium, N,N'-diethyl-N-[6-(ethyldipropylammonio)hexyl]-N,N',N'-tripropyl-, triiodide (9CI) (CA INDEX NAME)



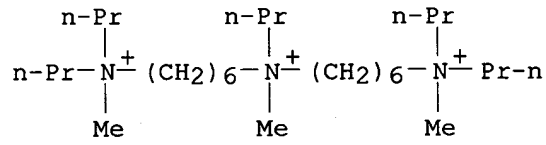
●3 I^-

RN 1862-38-0 CAPLUS
CN 1,6-Hexanediaminium, N,N,N,N',N'-pentapropyl-N'-[6-(tripropylammonio)hexyl]-, triiodide (9CI) (CA INDEX NAME)



●3 I^-

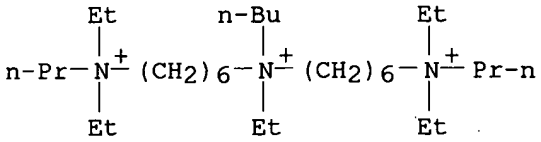
RN 4055-56-5 CAPLUS
CN Ammonium, [(methylpropyliminio)bis(hexamethylene)]bis[methyldipropyl-, triiodide (8CI) (CA INDEX NAME)



●3 I^-

RN 124245-58-5 CAPLUS
CN [(Butylimino)bis(hexamethylene)]bis[diethylpropylammonium iodide]

ethiodide (6CI) (CA INDEX NAME)



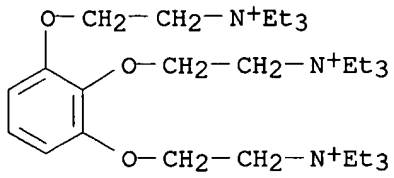
● 3 I^-

L17 ANSWER 35 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1960:39901 CAPLUS
DOCUMENT NUMBER: 54:39901
ORIGINAL REFERENCE NO.: 54:7895f-g
TITLE: Action of some **quaternary** ammonium base salts with curare-like activities upon the polarographic behavior of cystine
AUTHOR(S): Sherban, M.
SOURCE: Rev. chim. Acad. rep. populare Roumaine (**1959**), 4, 119-28
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB The following compds. with curare-like activity were investigated: d-tubocurarine, decamethonium, succinylcholine, flaxedil, and C100 (derivative of belladonna). The concentration of the curare-like compds. was kept at 10-5-10-4M while the concentration of cystine was maintained at 10-5M at pH 9.4.
The polarogram curves were traced at 3.8 v. and temperature 22°. Flaxedil was the most active. These **quaternary** compds. showed a pos. increase in the polarographic wave of cystine. The expts. indicated a close relation between the SH groups and the curare-like activities of compds. 13 references

IT **65-29-2**, Ammonium, [v-phenenyltris(oxyethylene)]tris[triethyl-iodide]
(effect on cystine polarography)

RN 65-29-2 CAPLUS
CN Ethanaminium, 2,2',2''-[1,2,3-benzenetriyltris(oxy)]tris[N,N,N-triethyl-, triiodide (9CI) (CA INDEX NAME)



● 3 I^-

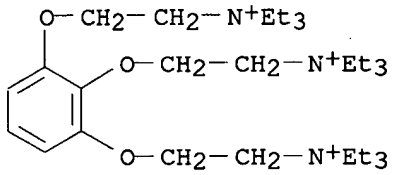
L17 ANSWER 36 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1959:119782 CAPLUS
DOCUMENT NUMBER: 53:119782

ORIGINAL REFERENCE NO.: 53:21361h-i,21362a
TITLE: Appearance of artifacts on chromatograms of **quaternary** ammonium compounds
AUTHOR(S): Crocker, Charity
CORPORATE SOURCE: Univ. Brazil, Rio de Janeiro
SOURCE: Journal of Chromatography (**1959**), 2, 115-16
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Choline chloride, hexamethylenebis(carbamoylcholine iodide) (606H.C.), 1,4-bis(2-piperidinoethyl)piperazinedi-EtI (336H.C.), and gallamine triethiodide (Flaxedil), each containing residual CCl3CO2H, showed the presence of artifact spots when chromatographed on paper in alkaline solvents. The size of the artifact spot increased at the expense of the principal spot with increasing amts. of CCl3CO2H. Solvent mixts. used were EtOH-NH3, PrOH-NH3-H2O, and BuOH-C5H5N-H2O. When the artifact was eluted and rechromatographed in the same solvent or in acid solvents, it reappeared as such and not as the parent **quaternary** ammonium compound

IT **65-29-2**, Ammonium, [v-phenenyltris(oxyethylene)]tris[triethyl-iodide]
(chromatography of, artifacts in)

RN 65-29-2 CAPLUS
CN Ethanaminium, 2,2',2''-[1,2,3-benzenetriyltris(oxy)]tris[N,N,N-triethyl-, triiodide (9CI) (CA INDEX NAME)



●3 I^-

L17 ANSWER 37 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1959:50670 CAPLUS
DOCUMENT NUMBER: 53:50670
ORIGINAL REFERENCE NO.: 53:9032c-i,9033a
TITLE: Neuromuscular blocking agents. II. A series of N,S,N-and N,N,N-trisethonium compounds
AUTHOR(S): Edwards, D.; Lewis, J. J.; Stenlake, J. B.; Zoha, M. S.
SOURCE: Journal of Pharmacy and Pharmacology (**1958**), 10, 106T-121T
CODEN: JPPMAB; ISSN: 0022-3573
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

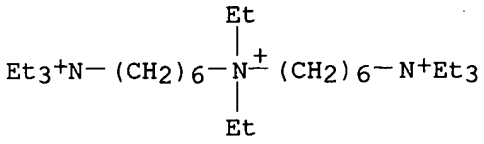
AB cf. C.A. 52, 8036f. 6-Hydroxyhexyldiethylamine (35.2 g.) in 95 ml. 48% HBr and 33 ml. H2SO4 was refluxed 4 hrs., cooled, poured into 1 l. H2O, Na2CO3 added and the mixture extracted with CHCl3, and the dried extract (Na2SO4) evaporated in vacuo to obtain crude 6-bromohexyldiethylamine (I) as a reddish brown oil containing crystalline material. The I obtained and 40 ml. ethylamine refluxed 2 hrs. and EtNH2 and CHCl3 evaporated yielded a damp crystalline mass;

this basified, extracted with, Et2O, and the extract evaporated yielded 24.8 g. oil,
distilled to yield 53% 6-ethylaminohexyldiethylamine (II), b0.55 86-9°, n17D 1.4493; di-HCl salt m. 172-3° (EtOH-Et2O). Crystalline material separated from crude II was 1,1-diethyl-1-azacycloheptylinium bromide, m. 250° (decomposition) (EtOH-Et2O). II and 6-chlorohexyldiethylamine refluxed in xylene 5 hrs. formed 19% bis(6-diethylaminohexyl)ethylamine, pale yellow oil, b0.7 165-8°, n18D 1.4610; this was refluxed 10 min. with EtI to form 7,7-diethyl-7-azoniatridecylenebis(triethylammonium) triiodide, m. 261-2°, needles (EtOH). Bis(10-diethylaminodecyl) sulfide was refluxed with EtI to form 27% 11-ethyl-11-thioniaheneicosylenebis(triethyl ammonium) triiodide, m. 123.5-24°, needles (Me2CO-Et2O). 10-Bromodecyldiethylamine (84%), b0.5 130°, n14D 1.4717, was obtained as an oil by the method for I. 10-Ethylaminodecyldiethylamine (76%), an oil, b0.8 133-5°, n18D 1.4535; di-HCl salt m. 147-8° (EtOH-Et2O). Bis(10-diethylaminodecyl)ethylamine (26.5%), pale yellow oil, b0.25 212-16°, n14D 1.4660; tri-HCl salt, m. 118° (Me2CO-Et2O). 11,11-Diethyl-11-azoniaheneicosylenebis(triethy lammonium) triiodide (90%) m. 202.5-3.5° (Me2CO-Et2O). 1,1-Bis(ethoxycarbonyl)-7-diethylaminoheptane (47.65%), pale yellow oil, b0.8 147-55°, n15.5D 1.4472, was used to prepare 62% Et 8-diethylaminocaprylate (III), an oil, b0.65 111-14°, n18D 1.4428; this reacted with EtI to form 7-ethoxycarbonylheptyltriethylammonium iodide, m. 64.5-5.5° (Me2CO-Et2O). III was reduced with LiAlH4 to obtain 90% 8-hydroxyoctyldiethylamine, an oil, b0.7 114-17°, n16.5D 1.4590; HCl salt m. 90-1° (EtOH-Et2O). 8-Chlorooctyldiethylamine (96%), an oil, b0.55 94-6°, n17D 1.4550 (literature, b11 130.5°, n18D 1.4535). Bis(8-diethylaminooctyl) sulfide (72%), straw-colored liquid, b0.65 210-12°, n18.5D 1.4768; di-HCl salt m. 145° (EtOH). 9-Ethyl-9-thioniaheptadecylenebis(triethylammonium) triiodide (47%) m. 159-60° (decomposition) (EtOH-Et2O). 8-Ethylaminooctyldiethylamine (76%), an oil, b0.7 104-6°, n17.5D 1.4530; di-HCl salt, hygroscopic, m. 159.5-60.5° (EtOH-Et2O). Bis(8-diethylaminooctyl)ethylamine (18%), yellow oil, b0.8 230-50°, n17D 1.4642; tri-HCl salt m. 165-6° (decomposition) (Me2CO-Et2O). 9,9-Diethyl-9-azoniaheptadecylenebis(triethylammonium) triiodide m. 251-2° (decomposition) (EtOH). 7-Dioxothiatridecylenebis(triethylammoni um iodide) (47%), pale buff solid, m. 144-5° (Me2CO-Et2O). All the compds. tested showed neuromuscular blocking activity. Dihexazonium triethiodide and the sulfone 7-dioxathiatridecylenebis(triethylammonium iodide) (dihexone) showed tubocurarinelike activity; dioctasulfonium and dioctazonium triethiodides were predominantly tubocurarinelike but had some transitional properties. Didecasulfonium and didecazonium triethiodides resembled decamethonium. Dihexazonium triethiodide was equipotent with tubocurarine on the cat. Marked species variations in potency were noted.

IT **3756-18-1**, Ammonium, [(ethylimino)bis(hexamethylene)]bis[triethyl- iodide], ethiodide **15159-46-3**, Ammonium, [(ethylimino)bis(octamethylene)]bis[triethyl- iodide], ethiodide **102031-41-4**, Ammonium, decamethylenebis[(10-diethylaminodecyl)diethyl- iodide], diethiodide **106715-64-4**, Ammonium, hexamethylenebis[(6-diethylaminohexyl)diethyl- iodide], diethiodide **108019-73-4**, Ammonium, [(ethylimino)bis(decamethylen e)]bis[triethyl- iodide], ethiodide
(preparation of)

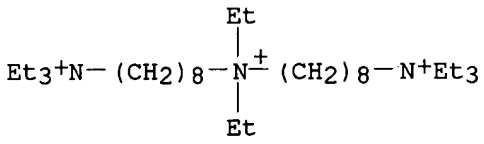
RN 3756-18-1 CAPLUS

CN 1,6-Hexanediaminium, N,N,N,N',N'-pentaethyl-N'-[6-(triethylammonio)hexyl]-, triiodide (9CI) (CA INDEX NAME)



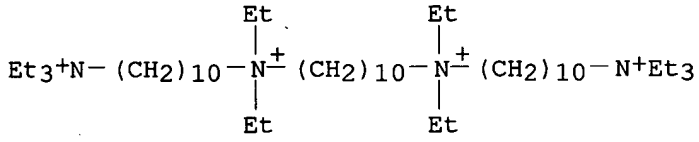
●3 I^-

RN 15159-46-3 CAPLUS
CN 1,8-Octanediaminium, N,N,N,N',N'-pentaethyl-N'-[8-(triethylammonio)octyl]-, triiodide (9CI) (CA INDEX NAME)



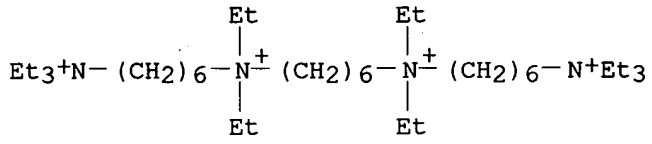
●3 I^-

RN 102031-41-4 CAPLUS
CN 3,3,14,14,25,25,36,36-Octaethyl-3,14,25,36-tetraazoniaoctatriacontane tetraiodide (6CI, 7CI) (CA INDEX NAME)



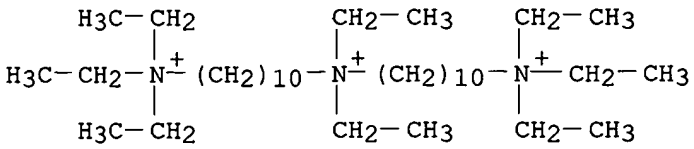
●4 I^-

RN 106715-64-4 CAPLUS
CN 3,3,10,10,17,17,24,24-Octaethyl-3,10,17,24-tetraazoniahexacosane tetraiodide (6CI, 7CI) (CA INDEX NAME)



●4 I^-

RN 108019-73-4 CAPLUS
CN 3,3,14,14,25,25-Hexaethyl-3,14,25-triazoniaheptacosane triiodide (7CI) (CA INDEX NAME)



●3 I^-

L17 ANSWER 38 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1958:89882 CAPLUS
DOCUMENT NUMBER: 52:89882
ORIGINAL REFERENCE NO.: 52:15830a-g
TITLE: Isolation, characterization, and determination of basic organic active substances of various medicinals with disulfimides. I
AUTHOR(S): Runge, F.; Engelbrecht, H. J.; Franke, H.
CORPORATE SOURCE: Univ. Halle, Saale, Germany
SOURCE: Pharmazie (**1957**), 12, 8-13
CODEN: PHARAT; ISSN: 0031-7144
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

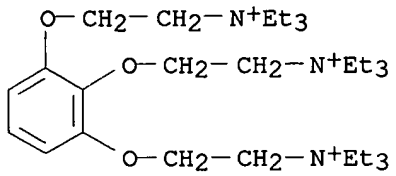
AB cf. C.A. 50, 7803h. The disulfimides (I) as strong acids form with organic bases crystalline salts poorly soluble in water. The most useful I is (4-ClC6H4SO2)2NNa (II), prepared by mixing NH4Cl and p-ClC6H4SO2Cl in Me2CO, adding 30% NaOH solution, and heating gently to distil off the Me2CO. The base (IIA) is prepared by dissolving II in hot water and precipitating with HCl, dissolving in anhydrous Et2O, evaporating, and crystallizing from C6H6. IIA, m. 205-6°, is well suited for the isolation, characterization, and determination of primary, secondary, tertiary, and **quaternary** amines, preferable often to picric acid or perchlorates, and especially for the **quaternary** compds., with which they form stable crystalline compds. with sharp m.ps. The amine or its salt combines with I or their alkaline salts in an ionic reaction. The free base in Et2O solution may be left to react with I directly, or I Na is mixed in aqueous, alc., or Me2CO solution with the **quaternary** base or its salts, advantageously with heat. An excess of either component retards crystallization, hence molar proportions must be used as closely as possible. The following medicinals were crystallized (compound and m.p. of product with IIA (uncorrected) given): anesthesine 150-1°; procaine 141-2°; 2-diethylaminoethanol 76-7°; coramine 153-4°; dilatol [1-(p-hydroxyphenyl)-2-(1-methyl-3-phenylpropylamino)propanol-HCl] 175-6°; sympathol 168-9°; dispasmol (N-benzyl-N',N'-dimethyl-N-phenylethylenediamine) 141-2°; rodismin (N-benzyl-N',N'-diethyl-N-phenylethylenediamine) 94-5°, 2-(α-phenyl-o-tolyloxy)triethylamine-HCl 128-9°; aminopyrine 167-8°; megaphen from 50° (unsharp); sulfanilamide 197-8°; sulfapyridine 165-6°; sulfacetamide Na, yellow crystals 167-8°; sulfaguanidine 108-9°; elkosin 179-80°; nicotinic acid hydrazide from 206° (decompose); tetramethyldecamethylenediamine-di-MeBr 150-1°; flaxedil 62-4°; choline chloride succinate 78-80°; hexamethonium bromide 214-15°; benzedrine 182-3°; thiamine-HCl 206-7°; niacinamide 212-14°; 3-pyridyl benzyl carbonate,

weak rose-colored needles, 167-8°; atrophan, yellowish needles, 171-2°; urotropine 162-3°; ephedrine 184-5°; atropine 145-6°; hyoscyamine 123-5°; papaverine 118-19° (unsharp); hydrastinine 139-40°; and yohimbine 196-7°. To determine satisfactory methods for gravimetric analysis, various I salts of 2 medicinals were prepared Thus, for casantin, were prepared compds. with (4-H2NC6H4SO2)2NH (m. 202-3°), II (m. 111-12°), and (3,4-Cl2C6H3SO2)2NH (III) (m. 146-7°). The last compound was found best because it had the lowest solubility, was well crystallized, and had a high mol. weight For hexamethonium bromide, salts were prepared with II (m. 214-15°) and with III (m. 207-8°). Gravimetric detns. for both compds. were more accurate than volumetric (argentimetric) detns. 11 references.

IT **65-29-2**, Ammonium, [v-phenenyltris(oxyethylene)]tris[triethyl-iodide]
(detection of, and preparation of its salt with 4,4'-dichlorodibenzenesulfonamide)

RN 65-29-2 CAPLUS

CN Ethanaminium, 2,2',2''-[1,2,3-benzenetriyltris(oxy)]tris[N,N,N-triethyl-, triiodide (9CI) (CA INDEX NAME)



● 3 I^-

L17 ANSWER 39 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1958:78488 CAPLUS

DOCUMENT NUMBER: 52:78488

ORIGINAL REFERENCE NO.: 52:13971a-c

TITLE: Influence on the metabolism of the eggs of Psammechinus microtuberculatus of **quaternary** ammonium compounds and phenothiazine derivatives

AUTHOR(S): Hofmann, H.

CORPORATE SOURCE: Friedrich Schiller Univ., Jena, Germany

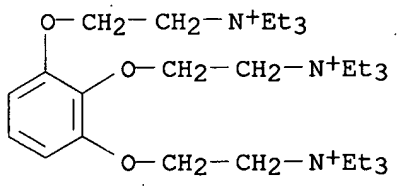
SOURCE: Pharmazeutische Zentralhalle fuer Deutschland (**1957**), 96, 421-31
CODEN: PHZEAD; ISSN: 0369-9773

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

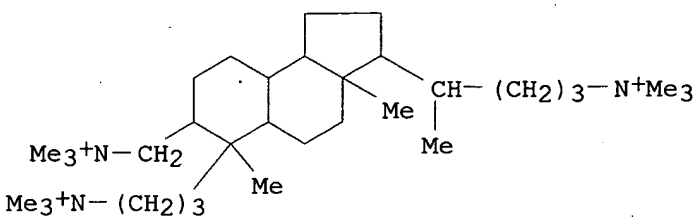
AB **Quaternary** ammonium compds. (d-tubocurarine chloride, Flaxedil, hexamethonium, decamethonium, and pendiomid) decreased the O consumption of fertilized and unfertilized eggs of R. microtuberculatus. The decrease in metabolism was inversely proportional to drug concentration Phenothiazine derivs. of the chlorpromazine type decreased the O consumption of sea-urchin eggs; above a certain limiting concentration the decrease in metabolism rose sharply and led to complete inhibition of oxidation. When combined with ethylurethan (I) the **quaternary** ammonium compds. showed an additive effect. The combination of phenothiazine derivs. and I gave a potentiating action. By this means, a further difference of the ganglioplegic drugs from the phenothiazine derivs. has been found.

IT **65-29-2**, Ammonium, [v-phenenyltris(oxyethylene)]tris[triethyl-iodide]
(inhibition of sea-urchin egg metabolism by)
RN 65-29-2 CAPLUS
CN Ethanaminium, 2,2',2''-[1,2,3-benzenetriyltris(oxy)]tris[N,N,N-triethyl-, triiodide (9CI) (CA INDEX NAME)



●3 I^-

L17 ANSWER 40 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1958:50718 CAPLUS
DOCUMENT NUMBER: 52:50718
ORIGINAL REFERENCE NO.: 52:9173i,9174a-c
TITLE: Multivalent **quaternary** ammonium compounds. VI. Some reaction products of bile acids and sterols
AUTHOR(S): Lettre, H.; Gottstein, W.; Scholtissek, Ch.
CORPORATE SOURCE: Univ. Heidelberg, Germany
SOURCE: Monatshefte fuer Chemie (**1957**), 88, 715-20
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C.A. 51, 4409a. Some N derivs. of lithiobilianic acid (I) and sitosterol are prepared I is treated with Ac2O followed by Me2NH to yield lithiobilianic acid 3-monodimethylamide, m. 251-2°. I with Ac2O followed by PCl5 and then with Me2NH in Et2O gives an Et2O phase containing 60%-70% I 3,4,24-tris(dimethylamide), m. 151-2°, purified by chromatography on Al2O3. The aqueous phase of the reaction yields 15-20% of I 3,24-bis(dimethylamide) (II), m. 232-3°. II is esterified with CH2N2 and reduced with LiAlH4 in tetrahydrofuran to 3,4-secocholan-4-ol-3,24-bis(dimethylamine hydrochloride), m. 292-5° (decomposition). II is similarly reduced to 90% 3,4-secocholane-3,4,24-tris(dimethylamine hydrochloride), decompose 275°, which forms 3,4-secocholane-3,24-tris(trimethylammonium iodide), m. 290° (decomposition). The dicarboxylic acid of sitosterol (III), heated 2 hrs. with Ac2O gives 76% 2,3-secositostanol-2,3-dicarboxylic acid anhydride, m. 176°. III di-Me **ester** is reduced by LiAlH4 to 88% 2,3-secositostane-2,3-diol, m. 182-3° (MeOH). III with PCl5 and Me2NH yields by chromatography on Al2O3 48% 2,3-secositostane-2,3-dicarboxylic acid dimethylamide, m. 106-7°, reduced by LiAlH4 to 68% 2,3-secositostane-2,3-bis(dimethylamine hydrochloride), m. 326° (decomposition). This compound with MeI gives 2,3-secositostane-2,3-bis(trimethylammonium iodide), m. 323°.
IT **122387-46-6**, 3,4-Secocholane-3,4,24-triamine, N3,N3,N4,N4,N24,N24-hexamethyl-, trimethiodide
(preparation of)
RN 122387-46-6 CAPLUS
CN 3,4-Secocholane-3,4,24-triamine, N3,N3,N4,N4,N24,N24-hexamethyl-, trimethiodide (6CI) (CA INDEX NAME)



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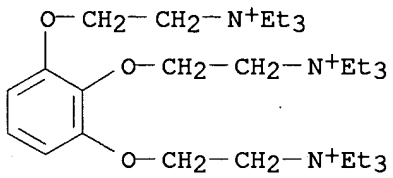
L17 ANSWER 41 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1957:6726 CAPLUS
DOCUMENT NUMBER: 51:6726
ORIGINAL REFERENCE NO.: 51:1456g-i
TITLE: Antagonists to the neuromuscular block produced by Sarin
AUTHOR(S): Kunkel, A. M.; Wills, J. H.; Monier, J. S.
CORPORATE SOURCE: Army Chem. Center, MD
SOURCE: Proceedings of the Society for Experimental Biology and Medicine (**1956**), 92, 529-32
CODEN: PSEBAA; ISSN: 0037-9727
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Large i.v. doses of Sarin decrease the twitch height of the cat gastrocnemius-soleus muscle group excited by maximal elec. stimulation of the sciatic nerve at 2-s. intervals. Various compds. containing **quaternary** N atoms, including several atropine derivs., overcome the decrease in twitch height. Some compds. with significant anticholinesterase activity enhance the Sarin-induced decrease in twitch height despite the abolition by Sarin of demonstrable cholinesterase activity in the muscle.

IT **65-29-2**, Ammonium, [v-phenenyltris(oxyethylene)]tris[triethyl-iodide]
(as antagonist for Sarin)
RN 65-29-2 CAPLUS
CN Ethanaminium, 2,2',2''-[1,2,3-benzenetriyltris(oxy)]tris[N,N,N-triethyl-, triiodide (9CI) (CA INDEX NAME)



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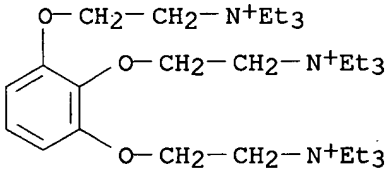
L17 ANSWER 42 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1952:6411 CAPLUS
DOCUMENT NUMBER: 46:6411

ORIGINAL REFERENCE NO.: 46:1150b-d
TITLE: Synthetic curarizing agents. III. Succinylcholine and its aliphatic derivatives
AUTHOR(S): Bovet, D.; Bovet-Nitti, F.; Guarino, S.; Longo, V. G.; Fusco, R.
CORPORATE SOURCE: Ist. super. sanita, Rome
SOURCE: Archives Internationales de Pharmacodynamie et de Therapie (**1951**), 88, 1-50
CODEN: AIPTAK; ISSN: 0003-9780
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 44, 1603c. Succinylcholine diiodide produces typical curarization in frogs and mammals. Birds, and the isolated frog rectus abdominis, show a nicotine-like contracture. In the dog, there is no effect on the blood pressure or cardiac rhythm except in large doses when the drug causes hypertension and tachycardia. Excess salivation and bronchial secretion occur. The direct excitability of the gastrocnemius muscle is not affected. In the series X(R)3N(CH2)nOOC(CH2)mCOO(CH2)nN(R)3 X the curarizing action is most marked if a chain of about 10 C and O atoms separate the **quaternary** nitrogens, and the substituent groups on the N are Me. Some of the series I(CH3)3N(CH2)5COOCH2CH2N(CH3)3 I, and the series I(CH3)3NCH2CH2OOC(CH2)2COOCH2CH2N(CH3)3 I are also active, but branching of the chain or the introduction of a third or fourth **quaternary** N destroys the activity.

IT **65-29-2**, Ammonium, [v-phenenyltris(oxyethylene)]tris[triethyl-iodide]
(pharmacology of)

RN 65-29-2 CAPLUS
CN Ethanaminium, 2,2',2''-[1,2,3-benzenetriyltris(oxy)]tris[N,N,N-triethyl-, triiodide (9CI) (CA INDEX NAME)



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L17 ANSWER 43 OF 43 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1948:1255 CAPLUS
DOCUMENT NUMBER: 42:1255
ORIGINAL REFERENCE NO.: 42:274a-g
TITLE: Curarizing properties of phenolic ethers with **quaternary** ammonium groups
AUTHOR(S): Bovet, Daniel; Depierre, France; de Lestrange, Yvonne
SOURCE: Compt. rend. (**1947**), 225, 74-6
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

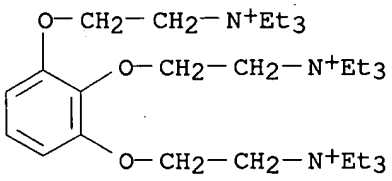
AB A study was made of the action on striated muscle of synthetic curarizing agents consisting of ethers formed from choline and homologous amino alcs. with phenols and polyphenols. The following compds. were used: C6H5OCH2CH2N(CH3)3I (I), 1,3-C6H4[OCH2CH2N(CH3)3I]2 (II), C6H5OCH2N(C2H5)3I (III), 1,2-C6H4[OCH2CH2N(C2H5)3I]2 (IV), 1,3-C6H4[OCH2CH2N(C2H5)3I]2 (V), 1,4-C6H4[OCH2CH2N(C2H5)I3I]2 (VI),

1,2,3-C6H3[OCH2CH2N(C2H5)3I]3 (VII). In the choline series, I and II were effective in the rabbit in doses of 4 mg. per kg. given intravenously. In the triethylcholine series, III has very slight activity, but IV, V, VI, and especially VII, are very active, the last causing curarization of 3 hrs. duration in the rabbit, in a dose of 0.7 mg. per kg. In the **quaternary** amines, choline and the **ester** salts of choline, particularly acetylcholine and butyl-β-ethylcholine (Dale, C.A. 9, 104) the curarizing effects seem to be closely connected with other cholinergic, muscarinic, and nicotinic manifestations of the mol. It was observed that in the ethers of the polyphenols studied, the cardiovascular effects are considerably attenuated. While I causes hypertension comparable to that produced by nicotine, II exerts only a weak nicotinic action. Likewise, the hypotensive and cardiomoderating effect of III is considerably weakened by the introduction of 1 or 2 more **quaternary** ammonium groups. The effects of VII are particularly striking. This compound is very active in the frog, which is immobilized by it in doses of 10 mg. per kg. In the mouse, the toxic doses are 5.5, 15, and 425 mg., given intravenously, subcutaneously, and per os. In the rabbit, the toxic dose is 0.7 mg. given intravenously, and 2-3.5 mg. per kg. subcutaneously. This represents about 5 times the activity of tubocurarine. In a rabbit given artificial respiration, total paralysis lasts 2.5 hrs. with a dose of 7 mg. and 6 hrs. after 35 mg. To kill a rabbit under these conditions, 350 mg., or about 500 times the toxic dose is necessary. In the chloralosed dog given O by tracheal catheter, the response of the gastrocnemius muscle to elec. excitation at the peripheral end of the sciatic nerve decreases in amplitude, then disappears at the same time as paralysis of the respiratory muscles occurs. The vagus is paralyzed, presumably at the synapses of its cardiac ganglia, but acetylcholine still exerts a large part of its normal effect. The injection of eserine (1-2 mg. per kg. in the atropinized dog) or of prostigmine, results in rapid recovery of muscular excitability. Injection of a dose of VII sufficient to cause curarization for several hrs. has no effect on blood pressure. In this respect the compound is superior to natural curare.

IT **65-29-2**, Ammonium, [v-phenenyltris(oxyethylene)]tris[triethyl- iodide]
(curarizing action of)

RN 65-29-2 CAPLUS

CN Ethanaminium, 2,2',2''-[1,2,3-benzenetriyltris(oxy)]tris[N,N,N-triethyl-, triiodide (9CI) (CA INDEX NAME)



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